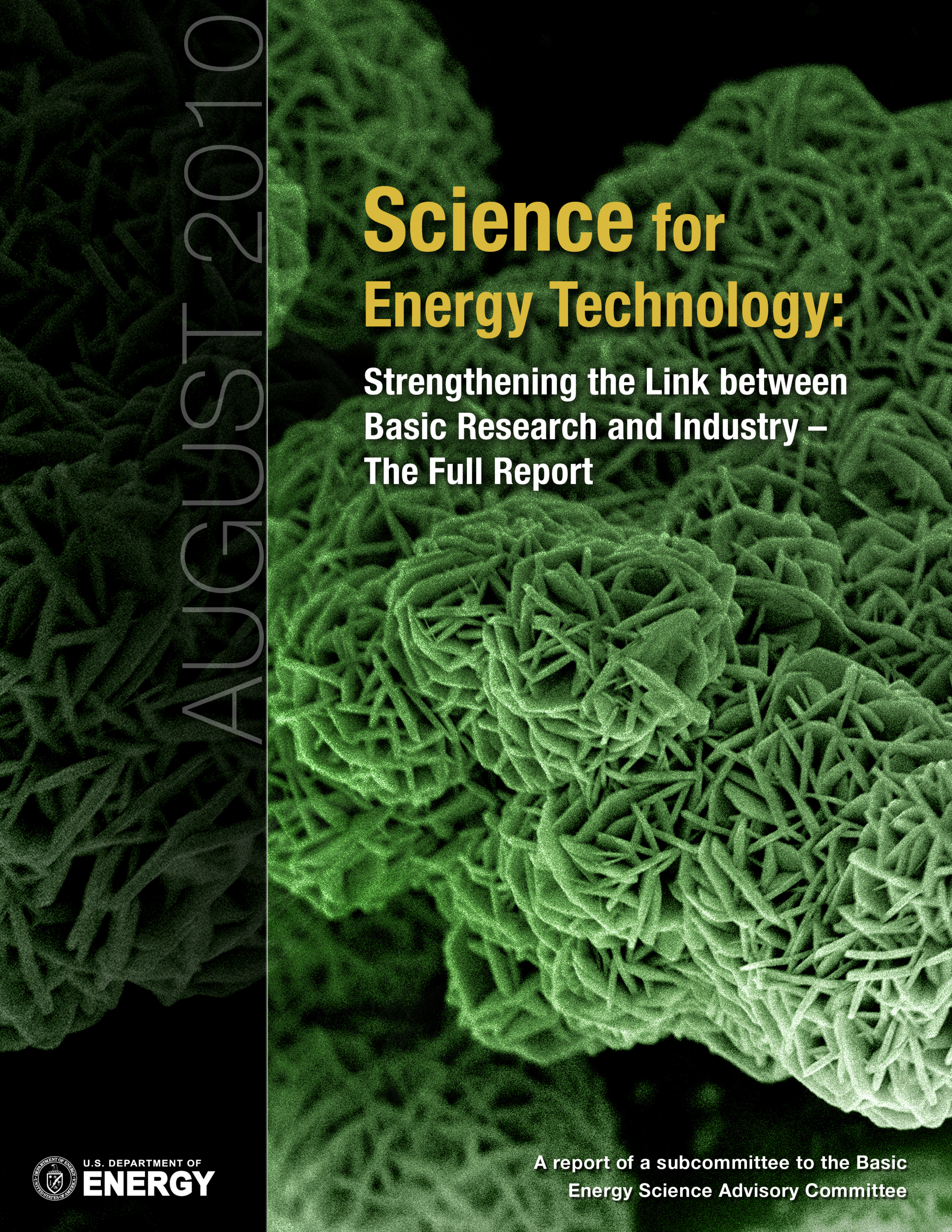


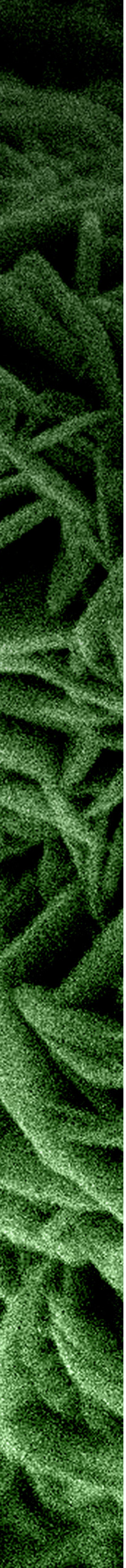
AUGUST 2010

Science for Energy Technology:

Strengthening the Link between Basic Research and Industry – The Full Report

U.S. DEPARTMENT OF
ENERGY

A report of a subcommittee to the Basic
Energy Science Advisory Committee



About the Department of Energy's Basic Energy Sciences Program

Basic Energy Sciences (BES) supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. This research provides the foundations for new energy technologies and supports DOE missions in energy, environment, and national security. The BES program also plans, constructs, and operates major scientific user facilities to serve researchers from universities, national laboratories, and private institutions.

About the "Basic Research Needs" Report Series

Over the past eight years, the Basic Energy Sciences Advisory Committee (BESAC) and BES have engaged thousands of scientists from academia, national laboratories, and industry from around the world to study the current status, limiting factors, and specific fundamental scientific bottlenecks blocking the widespread implementation of alternate energy technologies. The reports from the foundational Basic Research Needs to Assure a Secure Energy Future workshop, the following ten "Basic Research Needs" workshops, the panel on Grand Challenge science, and the summary report New Science for a Secure and Sustainable Energy Future detail the key basic research needed to create sustainable, low carbon energy technologies of the future. These reports have become standard references in the scientific community and have helped shape the strategic directions of the BES-funded programs. (http://www.sc.doe.gov/bes/reports/list.html)

1. Science for Energy Technology: Strengthening the Link between Basic Research and Industry
2. New Science for a Secure and Sustainable Energy Future
3. Directing Matter and Energy: Five Challenges for Science and the Imagination
4. Basic Research Needs for Materials under Extreme Environments
5. Basic Research Needs: Catalysis for Energy
6. Basic Research Needs for Electrical Energy Storage
7. Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems
8. Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels
9. Basic Research Needs for Advanced Nuclear Energy Systems
10. Basic Research Needs for Solid-State Lighting
11. Basic Research Needs for Superconductivity
12. Basic Research Needs for Solar Energy Utilization
13. Basic Research Needs for the Hydrogen Economy
14. Basic Research Needs To Assure A Secure Energy Future

About this Report

On January 18-21, 2010, approximately 100 experts representing a broad cross-section from industry, national labs, and academia came together at a BESAC-sponsored workshop to identify basic science efforts and Priority Research Directions for accelerating the development and growth of clean energy technology. Particular attention was given to identifying industry needs and the impact of basic science, of the type addressed by DOE's Office of Basic Energy Sciences (BES), in resolving the show-stoppers to industry progress.

On the cover:

Scanning Electron Microscope (SEM) image of self-assembled nanoplates of $(Ni_{4/9}Co_{1/9}Mn_{4/9})(OH)_2$, a precursor for growth of the new lithium-ion battery cathode material containing a $Li(Ni_xCo_yMn_{1-x-y})O_2$ component with high rechargeable energy density and a Li_2MnO_3 component providing improved stability. These mixed materials have the potential to raise the rechargeable energy density of the cathode by more than 50% while providing greater safety than the present cathodes based on $LiCoO_2$. Scale: each nanoplate is ~ 100 nm in thickness. S.-H. Kang, V. G. Pol, I. Belharouak, and M. M. Thackeray, Journal of the Electrochemical Society 157, A267-271 (2010). Source: Sun-Ho Kang and Vilas G. Pol, Argonne National Laboratory

Science for Energy Technology: Strengthening the Link between Basic Research and Industry

A Report from the
Basic Energy Sciences Advisory Committee

Chair:
John C. Hemminger
University of California, Irvine

U.S. Department of Energy

August 2010

Prepared by the BESAC Subcommittee on
Science for Energy Technology

Co-chairs:
George Crabtree
Argonne National Laboratory
and
Alexis Malozemoff
American Superconductor Corporation

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Associate Director of Science for Basic Energy Sciences

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NOTATION

$	dollar
$/kAmp-meter	dollars per kiloAmp-meter
$/W	dollars per watt
$/Wh	dollars per watt-hour
¢	cents
μA	microampere
μm	micrometer or micron
A	ampere
ac	alternating current
ACCR	aluminum conductor composite reinforced
ACSR	aluminum conductor steel reinforced
ACSS	aluminum conductor steel supported
AFM	atomic force microscopy
Ah	ampere-hours
Al_2O_3	aluminum oxide (alumina)
AlF_3	aluminum fluoride
AlInGaP	aluminum indium gallium phosphide
ALS	Advanced Light Source
AMSC	American Superconductor Corporation
ARPA-E	Advanced Research Projects Agency–Energy
AVO	amplitude versus offset
B	billion
BES	Office of Basic Energy Sciences
BESAC	Basic Energy Sciences Advisory Committee
BRN	Basic Research Needs
BTU	British Thermal Unit
BWR	boiling water reactor
C	Celsius
CCS	carbon capture and storage
CIGS	copper-indium-gallium diselenide
cm	centimeter
cm^2	square centimeter
Co	cobalt
CO	carbon monoxide
CO_2	carbon dioxide
CRADA	Cooperative Research and Development Agreement
CRF	Combustion Research Facility
$Cr(OH)_3$	chromium hydroxide
CrO_3	chromium trioxide

$CrO_2(OH)_2$	dihydroxy(dioxo)chromium
CuO	copper oxide
CZTS	copper zinc tin sulfide
dc	direct current
DFT	density functional theory
DOE	U.S. Department of Energy
DOS	density of states
EDS	energy-dispersive X-ray spectroscopy
EERE	Office of Energy Efficiency and Renewable Energy
EFRC	Energy Frontier Research Center
EPA	Environmental Protection Agency
EU	European Union
eV	electron volt
EV	electric vehicle
Fe	iron
Fe_2P	iron phosphide
g	gram
GaN	gallium nitride
GDP	gross domestic product
GE	General Electric
GHG	greenhouse gas
gpy	gallons per year
GW	gigawatt
H^+	hydron, hydrogen ion
HAADF-STEM	High-Angle Annular Dark-Field Scanning Transmission Electron Microscopy
HEV	hybrid electric vehicle
HTS	high-temperature superconductor
HV	high-voltage
IGBT	Insulated Gate Bipolar Transistor
IP	intellectual property
IPFC	Interline Power Flow Controller
IV	Current-voltage
J-V	current density-voltage
K	Kelvin
kV	kilovolt
kW	kilowatt
kWh	kilowatt-hour

$LaCrO_3$	lanthanum chromite
LDRD	laboratory-directed research and development
LED	light-emitting diode
Li	lithium
Li-ion	lithium ion
$LiB(C_2O_4)$	Lithium bis(oxalato)borate
$LiBH_4$	Lithium borohydride
LiBOB	Lithium bis(oxalato)borate
$LiCoO_2$	lithium cobalt spinel
$LiCoPO_4$	lithium cobalt phosphate
$LiFePO_4$	lithium iron phosphate
$LiMn_2O_4$	lithium manganese spinel
$LiMnPO_4$	lithium manganese phosphate
$LiNiO_2$	lithium nickel oxide
$Li_2O \cdot 2B_2O_3$	lithium diborate
$LiPF_6$	lithium hexafluorophosphate
$LiTi_2O_4$	lithium titanium oxide
LPW	lumens per watt
LWR	light water reactor
m	meter
m^2	square meter
MCFC	molten carbonate fuel cell
Mg	magnesium
MgB_2	magnesium diboride
MgO	magnesium oxide
mm	millimeter
mm^2	square millimeter
MM	million
Mn	manganese
$MnCr_2O_4$	manganese chromite
MoS_2	molybdenum disulfide
MOU	Memorandum of Understanding
MV	megavolt
MV/cm	megavolt per centimeter
MW	megawatt
NbTi	niobium titanium
Ni	nickel
Ni^{2+}	nickel ion
$NiCr_2O_4$	nickel chromite
NiMH	nickel-metal-hydride
NiO	nickel oxide
NiW	nickel tungsten
NMR	nuclear magnetic resonance
NO_x	oxides of nitrogen

NSLS	National Synchrotron Light Source
O^{2-}	oxygen ion
OE	Office of Electricity Delivery and Energy Reliability
OLED	organic light-emitting diode
oz	ounce
PAFC	phosphoric acid fuel cell
pcAFM	photoconductive atomic force microscopy
Pd	palladium
PEMFC	proton exchange membrane fuel cells
PHEV	plug-in hybrid electric vehicle
PIA	proprietary information agreement
PRD	priority research direction
Pt	platinum
PT	polythiophene
PV	photovoltaic
PVdF	polyvinylidene fluoride–hexafluoropropene
PWR	pressurized water reactor
R&D	research and development
Rh	rhodium
ROW	right-of-way
rpm	revolutions per minute
SEI	solid electrolyte interface
SEM	scanning electron microscope
SIMS	secondary ion mass spectrometry
SiO_2	silicon dioxide
SnO_2	tin dioxide
SOFC	solid oxide fuel cell
SRC	Semiconductor Research Corporation
SSL	solid-state lighting
SSSC	Static Synchronous Series Compensator
STATCOM	Static Synchronous Compensator
SUF	scientific user facility
SVC	Static VAR Compensator
T	Tesla
TCSC	thyristor-controlled series capacitor
TEM	transmission electron microscope/microscopy
TiO_2	titanium dioxide
TOF-SIMS	time-of-flight secondary ion mass spectrometry
TW	terawatt
TWh	terawatt-hour

UIC	Underground Injection Control (Program)
UPFC	Unified Power Flow Controller
USCAR	United States Council for Automotive Research
UV	ultraviolet
V	volt
VO_2	vanadium dioxide
W	watt
W/cm	watts per centimeter
Wh/kg	watt-hour per kilogram
Wh/l	watt-hour per liter
WO_3	tungsten trioxide
XPS	X-ray photoelectron spectroscopy
YBCO	yttrium barium copper oxide
ZrO_2	zirconium oxide

Executive Summary

The nation faces two severe challenges that will determine our prosperity for decades to come: assuring clean, secure and sustainable energy to power our world and establishing a new foundation for enduring economic and jobs growth. These challenges are linked: the global demand for clean sustainable energy is an unprecedented economic opportunity for creating jobs and exporting energy technology to the developing and developed world. But achieving the tremendous potential of clean energy technology is not easy. In contrast to traditional fossil fuel-based technologies, clean energy technologies are in their infancy, operating far below their potential, with many scientific and technological barriers to overcome.

Industry is ultimately the agent for commercializing clean energy technology and for reestablishing our economic and jobs growth. For industry to succeed in these challenges, it must overcome many roadblocks and continuously innovate new generations of renewable, sustainable, and low-carbon energy technologies such as solar energy, carbon sequestration, nuclear energy, electricity delivery and efficiency, solid state lighting, batteries and biofuels. The roadblocks to higher performing clean energy technology are challenges not just of engineering design but also of scientific understanding; innovation relies on contributions from basic research to bridge major gaps in our understanding of the phenomena that limit efficiency, performance, or lifetime of the materials or chemistries of these sustainable energy technologies. Thus, efforts aimed at understanding the scientific issues behind performance limitations can have a real and immediate impact on cost, reliability, and/or performance of a technology, and ultimately a transformative impact on our economy.

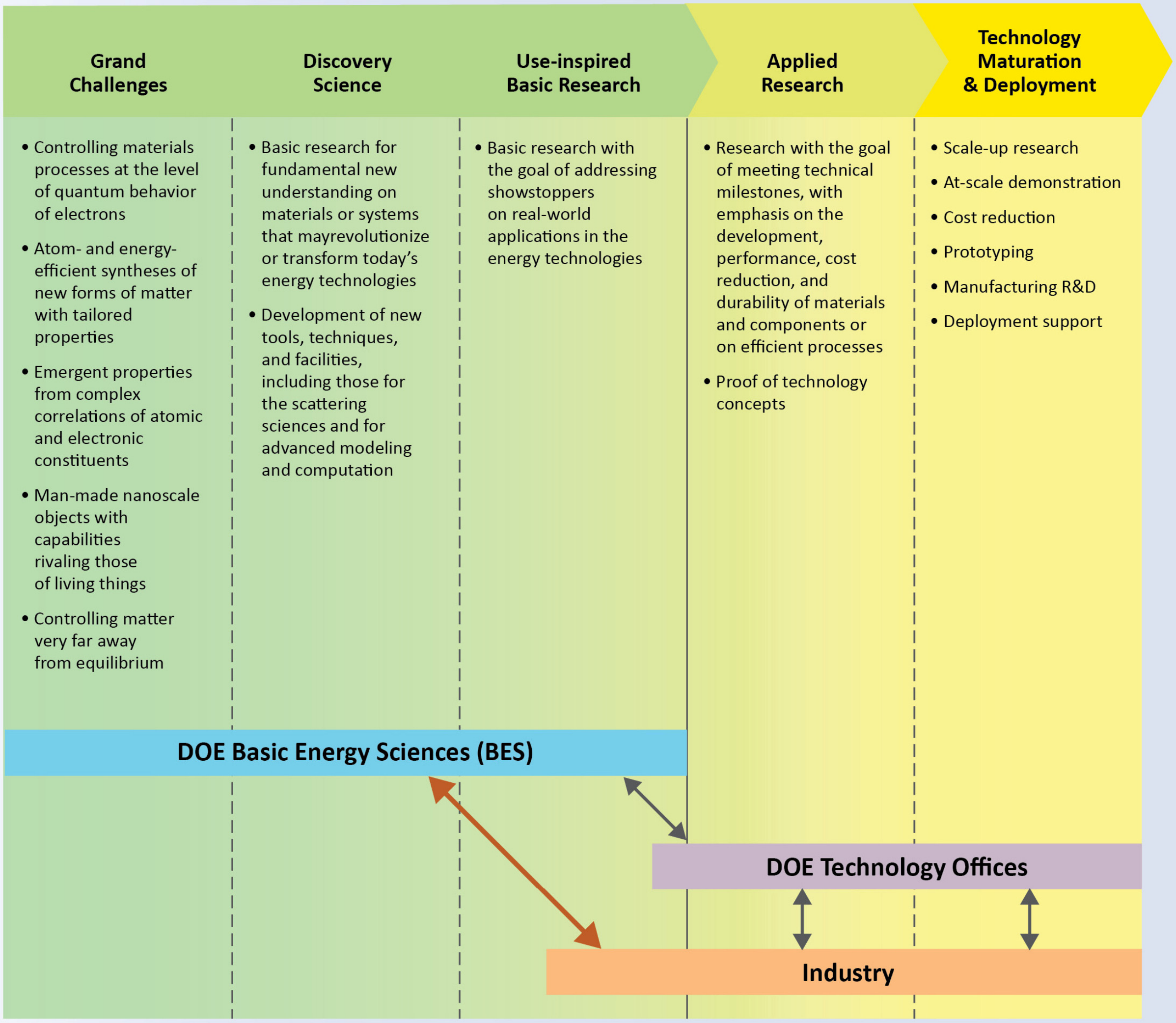
With its broad research base and unique scientific user facilities, the DOE Office of Basic Energy Sciences (BES) is ideally positioned to address these needs. BES has laid out a broad view of the basic and grand challenge science needs for the development of future clean energy technologies in a series of comprehensive Basic Research Needs workshops and reports (inside front cover and http://www.sc.doe.gov/bes/reports/list.html) and has structured its programs and launched initiatives to address the challenges.

The basic science needs of industry, however, are often more narrowly focused on overcoming specific nearer-term roadblocks to progress in existing and emerging clean energy technologies. To better define these issues and identify specific barriers to progress, the Basic Energy Sciences Advisory Committee (BESAC) sponsored the Workshop on Science for Energy Technology, January 18-21, 2010. A wide cross-section of scientists and engineers from industry, universities and national laboratories delineated basic science Priority Research Directions most urgently needed to address the roadblocks and accelerate the innovation of clean energy technologies. These Priority Research Directions address the scientific understanding underlying performance limitations in existing but still immature technologies. Overcoming these performance limitations can dramatically improve the commercial penetration of clean energy technologies

A key conclusion of the Workshop was that while the Basic Research Needs reports delineate decadal foundational challenges in the development of new energy technologies, specific basic research directions addressing nearer-term industry roadblocks are ripe for further emphasis. These priority research directions are detailed in the present report. Another key conclusion is that identifying and focusing on specific scientific challenges, and then translating the results to industry, requires more direct feedback, communication and collaboration between industrial and BES-supported scientists. BES-supported scientists need to be better informed of the detailed scientific and technological issues, and industry needs to be more aware of BES capabilities and how to utilize them. An important capability is the suite of BES scientific user facilities, which can play a key role in advancing the science of clean energy technology.

Working together, industry and BES-supported scientists can achieve understanding and control of the performance limitations of clean energy technology, translation of this knowledge to industry, and development of the workforce needed to build the growing clean energy technology economy.

The Energy Science and Technology Spectrum



Grand Challenges	Discovery Science	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment
• Controlling materials processes at the level of quantum behavior of electrons • Atom- and energy-efficient syntheses of new forms of matter with tailored properties • Emergent properties from complex correlations of atomic and electronic constituents • Man-made nanoscale objects with capabilities rivaling those of living things • Controlling matter very far away from equilibrium	• Basic research for fundamental new understanding on materials or systems that mayrevolutionize or transform today's energy technologies • Development of new tools, techniques, and facilities, including those for the scattering sciences and for advanced modeling and computation	• Basic research with the goal of addressing showstoppers on real-world applications in the energy technologies	• Research with the goal of meeting technical milestones, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes • Proof of technology concepts	• Scale-up research • At-scale demonstration • Cost reduction • Prototyping • Manufacturing R&D • Deployment support

To accelerate the innovation and development of critically needed energy solutions, effective communication is essential between, on one side, fundamental research developed in the DOE Office of Basic Energy Sciences and, on the other side, the applied community, in the DOE technology offices and in industry. Major opportunities exist to enhance the direct link between BES and industry (red arrow).

Chapter 1: Introduction

I. CONTEXT

Science supported by the U.S. Department of Energy (DOE) Office of Basic Energy Sciences (BES) has a critical role to play in addressing the enormous energy problems we face as a nation, indeed as a planet.

Energy demands worldwide, for electricity as well as transportation and heating fuels, are expected to double by 2050, raising critical energy supply issues. At the same time, levels of carbon dioxide and other greenhouse gases in the atmosphere are climbing inexorably, raising compelling environmental concerns. These and many related issues make it a national priority to achieve higher efficiency throughout our energy infrastructure, along with a massively larger role for renewables and a dramatic reduction in greenhouse gas emissions.

The importance of science in addressing these challenges can hardly be overstated. A suite of technologies is already in play addressing the challenges, but existing commercial technologies are clearly incapable of dealing in their present form with the magnitude of what needs to be accomplished. Transformative breakthroughs are required to address the full scope of the challenges, and such breakthroughs generally come from the discoveries and fundamental understanding that only scientific research can bring.

The DOE BES supports a broad spectrum of foundational basic research and is the single largest funder of fundamental energy science research in the United States. Through competitive peer review, it funds an extraordinary pool of researchers in national labs and academia, who provide a unique resource for addressing the science issues related to the energy challenges we face.

During the last seven years, a series of workshops has been held under the auspices of the Basic Energy Sciences Advisory Committee (BESAC) and BES. These workshops led to the “basic research needs” (BRN) reports (inside front cover and accessible at http://www.sc.doe.gov/bes/reports/list.html), which describe the many opportunities for transformative science to have an impact on the critical energy problems we face. The workshops brought together members of the international scientific community, including researchers and experts from national laboratories, academia, and industry.

These reports have already motivated a significant response from BES: the establishment of 46 Energy Frontier Research Centers (EFRCs), addressing many of the scientific topics relevant to our energy challenges. With an overall budget of $125M per year, the EFRCs are a major investment by DOE to accelerate scientific research in this important area. Other DOE initiatives, including the Advanced Research Projects–Energy (ARPA-E) and the Energy Innovation Hubs, have provided complementary resources across the continuum from fundamental science to technology deployment.

Nevertheless, the energy challenges we face are so critical that the question arises – is there more that can be done to accelerate progress? The BRN reports addressed primarily longer-term scientific directions, but beyond these, there is a need to identify scientific opportunities with nearer-term impact, especially those directly addressing industry needs and so enabling more rapid deployment of new technical solutions and products. What are the barriers to addressing such opportunities?

The purpose of this report, following on an earlier concept report (April 2010), is to address these issues.

II. BRINKMAN'S CHARGE

On July 1, 2009, Dr. William Brinkman, Director of the DOE Office of Science, issued a charge to the BESAC: prepare two new reports, a short high-level one with a less technical message, and another full report with more complete technical descriptions. The reports are to address the following three points:

1. Summarize science themes from the BRN reports, with emphasis on **needs of more applied energy technologies**, and identify grand challenge science drivers likely to have **near-term impact** in the energy arena.

2. Identify how the suite of BES-supported and -managed scientific **user facilities** can impact basic and applied research on energy.

3. Identify other major **impediments** to successful achievement and implementation of transformative energy technologies, including potential deficits in human capital and workforce development, and **possible solutions** to these problems.

These reports, which will "link basic research with applied problems in energy technologies," are expected to help guide the DOE BES and the DOE Office of Science in establishing future scientific directions to address the critical near-term energy technology issues that face the nation.

An important juxtaposition here is of the words "science" and "basic research" on the one hand, and "more applied energy technologies" on the other. Brinkman's charge raises a key question: is the kind of fundamental science addressed by BES-supported researchers as relevant as it could be to *applied* energy technologies? Once applied work is underway, hasn't the science part already been done? Actually in much industrial technology development, this is far from the case. Under competitive and commercialization pressures, industry more often than not forges ahead with empirical process and device optimization without establishing a full scientific understanding of the processes and phenomena involved. When empirical optimization reaches its limits, better scientific understanding is usually needed to break through the bottleneck and make further progress.

Another perhaps surprising juxtaposition is of the words "near term" and "transformative." Given the typically long-term timeline for science to address fundamental issues, are there *any* science opportunities that satisfy both of these apparently contradictory criteria? In fact, there are many such opportunities. These arise because many nascent technologies are already being developed in industry; they have a "head start." But they need better scientific understanding to make further breakthroughs and ensure broad, not just niche, impact. In many cases, a relatively modest further advance in cost and/or performance can bring a nascent technology across a competitive commercial threshold (the “tipping point”) and suddenly turn what was initially a niche product into one with transformative impact.

III. BESAC SUBCOMMITTEE AND WORKSHOP ON SCIENCE FOR ENERGY TECHNOLOGIES

In response to Brinkman’s charge, BESAC commissioned a Subcommittee on Science for Energy Technologies, chaired by Dr. George Crabtree of Argonne National Laboratory and Dr. Alexis Malozemoff of American Superconductor Corporation, with the responsibility of addressing Brinkman’s charge and developing the requested reports.

To establish and validate the link between basic research and applied problems, it is essential to obtain a clear picture of industry needs for basic research (i.e., technology pull rather than science push). Thus, the Subcommittee was populated principally with industrial members with expertise in various areas of energy technology as well as a good grounding in science. These were complemented by several “generalists” who brought a strong insight and awareness of the existing BRN reports and a background in national labs and academia. The members of the Subcommittee are listed at the front of this report.

Nine topical areas for the report were defined (see inside back cover); they correspond broadly to the BRN topics, although an effort was made to define the topical areas more on the basis of industry needs than on the basis of scientific area. For example, rather than have superconductivity as a topic, electricity delivery was chosen. Superconductivity represents one, but only one, of the scientific areas that can affect electricity delivery through high-temperature superconductor cables, current limiters, and so forth. Power electronics, dielectrics, and cryogenics are some others.

The list of topical areas is by no means complete; topics such as carbon capture (as distinct from carbon sequestration), advanced grid modeling, energy storage by other than electrochemical means, and aspects of the hydrogen economy other than fuel cells are not covered. These omissions should not be taken to imply anything about the importance of these areas as compared to the ones addressed here, and follow-up studies are encouraged to evaluate the scientific opportunities in these and other such areas.

To address the charge, the BESAC Workshop on Science for Energy Technologies, supported by BES, was held on January 18-21, 2010, at the Hilton Hotel in Rockville, Maryland, with about 100 participants, including the panel members listed in chapters of this report. Panels were convened in each of nine topical areas. For each panel, 5-10 participants were chosen to provide a broad cross section of experts from industry, national labs, and academia. The panels were instructed to respond to Brinkman’s charge by (1) identifying industry needs and priority research directions (PRDs) that met the charge guidelines, (2) identifying opportunities for BES-supported user facilities to make an impact, and (3) addressing other non-technical impediments with possible solutions. The outputs of these nine panels provide the basis for this full report and the brief high-level concept report issued by BESAC in April 2010.

IV. PRIORITY RESEARCH DIRECTIONS

A. Criteria Used in Selecting PRDs

To review such a vast range of topics, which had required ten separate BRN workshops to accomplish over seven years, the present Workshop needed to build on that previous work. Nevertheless, it was not simply a matter of repeating the conclusions of the earlier work, because the focus suggested by Brinkman was somewhat different, leading to three basic criteria used in selecting the PRDs:

1. *Address industry needs and national priorities*. The national priorities of increasing energy efficiency and use of renewables, of reducing greenhouse gases, and of ensuring a capable and stable electric power grid broadly cover all the topics of the Workshop. The industry needs for addressing these priorities were defined with the help of industry participants in the Workshop.

2. *Require meaningful science*. Although there are many definitions of "meaningful science," the Workshop focused on science probing the frontiers of human knowledge rather than applying well-established principles as in most engineering work. The PRDs were required to use the scientific method: a discipline including hypotheses, experimentation or simulation, and objective analysis of results. And they were required to be of significant and fundamental scope to differentiate them from what could be called "job shop" activity on technical issues of smaller scope for industry.

3. *Create an opportunity for near-term impact*. "Near term," another potentially ambiguous term, was defined by the organizers as a maximum of five years to a proof of principle which could be handed off to industry for product development, scale-up, and eventually manufacturing.

The above criteria were used to identify various PRDs, and additional criteria were applied to prioritize them:

1. *Degree of impact once technology is commercialized*. Clearly the high-priority PRDs need to target major areas with broad impact on energy efficiency, renewable energy, and greenhouse gas reduction.

2. *Probability of success*. Although science by its very nature is probing the unknown and is, therefore, intrinsically uncertain, the probability of success often grows with the degree to which other aspects of the problem have already been addressed. For example, work on some poorly understood aspects of known materials usually has a higher probability of success in a short time than the serendipitous search for a totally new material, which would subsequently require a decade or more to develop into a commercial product.

3. *Shorter timing*. The sooner the commercial impact on major energy challenges, the better.

Ultimately, workshop participants identified 26 PRDs central to near-term energy technology challenges. They are listed at the end of this report and are described in detail in the body of the report.

Many of these PRDs echo those identified earlier in BES-sponsored BRN workshops and reports (see inside front cover and www.sc.doe.gov/production/bes/reports/list.html). However, some of the Workshop research directions were entirely new, and most were directed to developing scientific understanding underlying the performance limitations in already existing and emerging clean energy technologies rather than on the longer-term search for entirely new materials or processes.

There is no question that BES should maintain its commitment to fundamental research, including long-term grand challenge research and discovery science (see figure preceding this chapter). At the same time, a key recommendation of this report is that BES should seek opportunities to improve existing mechanisms and develop new mechanisms to strengthen use-inspired research of interest to industry by addressing the PRDs identified here.

B. Overarching Themes

Several overarching themes, in addition to technology-specific roadblocks, emerged from the PRDs.

1. Research to develop foundational scientific understanding of at-scale production challenges in existing materials and processes for emergent energy technologies,

   for example, understanding loss processes that limit the efficiency of full-scale solar cells by as much as a factor of two compared to laboratory cells. Success in that endeavor could vault photovoltaic technology into cost-performance parity with fossil-fuel-based electric energy, enabling a vastly increased solar contribution to renewable energy and opening immense economic opportunities to export inexpensive solar technology to the world.

2. Research that extends beyond empiricism toward the fundamental understanding of lifetime prediction of materials in extreme environments, especially aging, degradation, and failure,

   for example, understanding degradation mechanisms under the extreme irradiation, thermal, and corrosive conditions of nuclear reactors. Success in that endeavor would enable improved prediction and certification of extended lifetimes for existing and future nuclear reactors, a critically important source for carbon-free baseload energy complementing the more variable renewable resources like solar and wind.

3. Research aimed at the discovery of specific new materials or chemical processes with targeted functionality that would lower the cost and improve the efficiency of clean energy technologies,

   for example, developing modeling frameworks to predict the performance of new biomass conversion catalysts in complex cellulosic mixtures. Success in that endeavor would enable a breakthrough in conversion of cellulosic biomass to fuels, supplementing or even displacing the present corn-starch-to-ethanol pathway and significantly reducing demand for oil.

C. Crosscutting Areas of Scientific Expertise

In addition to these common overarching themes, the PRDs revealed cross-cutting areas of scientific expertise required for success.

The challenge of creating new materials by design, with specific properties or functionalities, is ubiquitous. We need to use the enormously powerful computational capability now available to predict the properties of materials with complex atomic and nanoscale structures, so that we can design the structures with targeted functionality needed for a given energy technology. Part of this challenge is to model the properties on all length scales from nanometers to whatever macroscopic length scale is relevant for the particular technology. We then need to use directed synthesis and fabrication techniques to create the material with the predicted atomic, molecular, and microscopic structure, and test its functionality in applications using state-of-the-art characterization, such as scattering user facilities and benchtop scanning probes. This task is especially important and difficult for complex materials with multiple components and interfaces in device geometries.

Understanding and predicting the role of interfaces was a recurrent theme; advances in surface and interface science, broadly defined, are needed. Interfaces play a critical role in the optical, electrical, mechanical, and chemical properties of materials. For example, the efficiencies of solar cells and solid-state lighting are critically sensitive to the behavior of electrons at interfaces between semiconductors with different compositions. The stability of nuclear materials and the movement of carbon dioxide through rock for carbon sequestration depend on the mechanical and chemical properties of surfaces and grain boundaries.

The challenge of understanding and controlling dynamical processes across a wide range of timescales was also common, calling for expertise in modeling and measuring transport processes and chemical kinetics. For example, one needs to model mass transport and chemical kinetics on timescales from femtoseconds to hours for biofuel production; for carbon sequestration the timescales of importance extend to thousands of years. Many energy conversion phenomena take place far from equilibrium, a prominent theme of previous BES and BESAC workshops and reports.

Put simply, the materials and phenomena that are central to energy technology needs are neither static nor homogeneous. Rather, the dynamical processes and intrinsic heterogeneities that dominate complex materials and chemical processes must be understood to enable their more effective utilization. A scientific knowledge base in treating dynamical processes and disorder needs to be brought to bear on clean energy technology.

D. Main Themes and Recommendations

Several major themes and recommendations emerged from the Workshop:

Theme: Major opportunities do indeed exist for near-term and at the same time transformative impact of BES science on the critical energy challenges of our nation.

> ***Recommendation: BES should find means, as expeditiously as possible, to actively enhance use-inspired energy science research addressing the PRDs identified in this report.***

- As emphasized in a recent report of the American Energy Innovation Council ("*A Business Plan for America's Energy Future*, http://www.americanenergyinnovation.org/full-report), "in one realm central to America's economic, national security and environmental future, our commitment to innovation is sorely lacking: energy." They argue for a major additional investment in clean energy innovation, especially when compared to the investment the nation has made in other critical fields like pharmaceuticals, aerospace and defense, and computers and electronics.
- New initiatives focused on the PRDs are needed. However, the PRDs were chosen without regard to whether or not programs already exist on these topics. Prior to initiating new programs, it is recommended that BES review the scope and status of any existing programs, whether within BES or supported by other federal agencies or industry. We recommend that BES seize the opportunity presented by existing programs such as the EFRCs, as well as synergies with other DOE initiatives such as the Innovation Hubs and ARPA-E programs to address the PRDs.

Theme: Communication and collaboration with industry are essential.

A major theme which emerged from the Workshop was the importance of *direct* interactions between industry and BES-supported university and national lab researchers. This theme is discussed in detail in Chapter 2 of this report. In the context of the various types of research supported by BES, this interaction is illustrated by the red double-headed arrow in the figure preceding this chapter.

> ***Recommendation: BES should develop and encourage new modes of interaction with industry, both for communication and for collaboration (see Chapter 2).***

Theme: BES-supported scientific user facilities provide unique capabilities for advancing and accelerating energy-related research.

A detailed description of opportunities for contributions to PRDs by the scientific user facilities is given in Chapter 11 of this report.

> ***Recommendation: BES should enhance industrial outreach by the scientific user facilities and develop a sustained effort to both engage targeted industrial sectors and further enhance the capabilities they provide (see Chapter 11 for details).***

Theme: The U.S. workforce in energy-related user-inspired science needs to be strengthened and grown.

Recommendation: BES should foster efforts to enhance the energy science workforce pipeline, including exploring exchanges with industry focused on energy-related topics (see Chapter 2).

Chapter 2: Barriers and Solutions

A. Drivers for Engagement of Basic Researchers with Industry

A major theme that emerged from the Workshop was the importance of direct interactions between industry and basic scientists in universities and national laboratories for advancing science in the clean energy field.

Such interactions aid basic scientists in identifying the scientific opportunities that address industry needs. This is particularly important for near-term impact, since basic scientists can easily find themselves out of touch with the actual state-of-the-art industrial thinking and development. Similarly, scientists in industry may not be aware of rapidly evolving fundamental understanding of phenomena that could greatly impact products. Face-to-face interactions stimulate ideas and novel approaches on both sides, through the productive synergy of different perspectives. Industry can reach out for basic science support by making available unique industrial state-of-the-art materials, samples, and analytical and simulation tools. Effective collaboration bringing to bear the complementary capabilities, both intellectual and equipment-based, of a university or national lab on the one hand, and of industry on the other, is often the fastest — and sometimes the only — way to make progress on a given problem. And perhaps most important of all, the transfer of information to industry to accelerate product development and commercialization is enormously facilitated by ongoing interactions in which the participants know each other and understand each others' language.

B. Barriers to Engagement of Basic Scientists with Industry

At the same time, there are many barriers to such communication and collaboration. Terminology differences and lack of background knowledge are common obstacles. More fundamentally, significant cultural and incentive differences impede interactions. Communication channels are clouded by differing incentives and operating styles; basic scientists typically set priorities from the "bottom up" (scientific push), following the most compelling scientific opportunities as they arise. They emphasize understanding phenomena and strive to disseminate results quickly through publication. In contrast, industry often sets priorities from the "top down" (technological pull), based on its most critical needs for specific technologies, emphasizing materials and device performance results as higher priorities than understanding phenomena, and does not routinely share publicly its internally developed knowledge.

Another challenge among many industrial program managers, particularly with regard to possible interaction with basic scientists, is the need to appreciate what science really means; too often, the pressure to solve short-term issues leads them to seek what could be termed "job shop" activity rather than identifying the more fundamental issues, which require a truly scientific approach.

Continuity of support for collaborative programs is also critical to fostering a meeting of minds between basic scientists and industry. Precisely because of the importance of developing trust and common language, it is essential for such programs to continue without sudden interruptions and redirections.

C. The Intellectual Property Barrier

While the U.S. Department of Energy (DOE) Office of Basic Energy Science (BES) does not directly engage in negotiations involving intellectual property, it should be recognized that dealing with intellectual property issues effectively is an important element in fostering the kinds of industry/basic research collaborations encouraged in this report. This is a responsibility of the technology transfer staffs of universities and national laboratories that negotiate with industry teams, and often involves individual researchers whose intellectual property contributions are at stake.

With the passage of the University and Small Business Patent Procedures Act (commonly known as the Bayh-Dole Act) in 1980 and the Federal Tech Transfer Act in 1986, the responsibility for pursuing patent protection and active commercialization of research results arising from federal government research funding became a requirement of the acceptance of research funding for universities, small businesses, non-profits, and national laboratories. Since that time, there has been a tremendous growth of activity, whereby these parties seek to commercialize their intellectual property through various approaches including licenses, Cooperative Research and Development Agreements, spin-offs, and other entrepreneurial activities. This has transformed the innovation landscape in the United States, leading to the creation of new technologies, products, goods, and services, as well as providing monetary return to inventors and to the organization hosting the research. Over the last three decades, researchers and administrators at universities and national laboratories have grown much closer to industry and the marketplace through licensing and other commercialization processes, with tremendous successes — and some growing pains. However, Bayh-Dole can strain university-industry relations when it is applied by universities to privately funded rather than federally funded research, as it clouds IP ownership issues. This can inhibit successful commercialization of inventions and discourage such private funding.

In a collaborative activity, industry usually has a strong preference for securing exclusive license agreements for the intellectual property (IP) of any university or national lab partner. University or national laboratory decisions on granting exclusive vs. non-exclusive licenses are influenced by two factors: which type of licensing is most likely to lead to rapid commercialization, and which type of license appears to be in the public interest. This decision is technology- and IP-specific. A university or national laboratory may grant exclusive licenses when it believes that exclusivity provides the best commercialization pathway and most frequently, in the cases where exclusivity is necessary to induce the investments needed to for commercialization. The majority of licenses are non-exclusive or exclusive to a specific field of use.

Even though they have been never been exercised, license terms providing the U.S. Government with “march-in” rights in agreements with universities and national laboratories and other research institutions are often another point of contention, as march-in rights give the U.S. Government the right to take back rights in the licensed intellectual property and have the technology commercialized by another party, if the first party is not progressing to commercialization. From the federal government perspective, the prospect of march-in rights helps to ensure that inventions resulting from federal funding will be commercialized. In addition, under Bayh-Dole, licensees are required to “substantially manufacture in the United States” — a requirement that can potentially block the route to lowest-cost manufacturing, thus creating another point of contention in license negotiations.

Many research institutions cannot or may not wish to invest in the full expense of the patent application process without an identified commercial pathway. Licenses negotiated prior to patent filing can be difficult and are complicated by issues of non-disclosure, which can lead to the perception that universities or national laboratories are withholding information from industry as a bargaining chip. Further, commercial entities are often reluctant to pay upfront fees when they face other substantial commercialization costs. In addition, information may be withheld by the research institution while patents are being filed, to ensure their intellectual property position. The increasing use of provisional patent applications has helped to ease these situations. Provisional patent applications can be filed quickly, thereby enabling more rapid and open discussion of research results in the license negotiation process.

By the same token, industry protects its intellectual property carefully for competitive reasons. A strong temptation for industry in communication with academic researchers is to simply listen without reciprocating — i.e., to be recipients of information without disclosing anything substantive, creating a similar perception of not being forthcoming or fully open. An industrial concern is that in the open information environment of universities and some national laboratories, practices might not be in place — or sufficiently enforced — to ensure the control of sensitive information disclosed to them. Even more difficult and preferably avoided is the situation in which a researcher collaborates with multiple companies, creating the need for a “firewall” to separate proprietary information arising from multiple collaborators.

These issues take on a different character depending on the type of company involved. While a number of larger companies like General Electric and Applied Materials, both contributors to this report, play a major role in clean energy technology, the United States is particularly rich in smaller start-up companies which champion key new technologies (see, for example, Fig 2-1). Several are represented by panel members of this report, including American Superconductor, A123 and Verenium. Because these smaller companies lack the R&D facilities possessed by larger companies, their need for science support is particularly acute. Their urgent drive to move their technologies forward to commercialization often requires collaborative agreements to be executed within weeks, much shorter than the typical time scale for

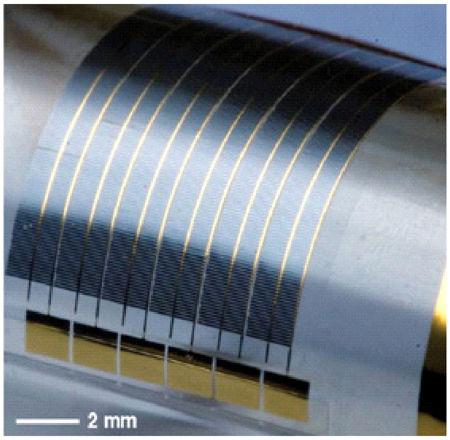


Figure 2-1 Flexible photovoltaic module composed of an interconnected array of hundreds of monocrystalline silicon microcells. This technology combines the attractive mechanical properties of organic devices with the lifetime and performance possible with inorganics [1]. The technology arose from basic research supported by BES at the University of Illinois Champaign-Urbana and was spun off through the startup company Semprius Corporation, supported by DOE-EERE. Source: John Rodgers, University of Illinois at Urbana-Champaign.

national laboratory and government decisions. Their limited venture capital or IPO funding, as well as their total focus on a single technology path, make IP issues critical to their success. In many cases, these companies have spun out of universities with an exclusively licensed patent to a breakthrough technology. However, as mentioned above, most clean energy technologies require multiple patents to bring to full commercial fruition. So license negotiations with third parties are critical to success, but start-up companies often lack the legal staff and experience to carry out these negotiations. On the other hand, they have the advantage of a compact executive structure which makes approval of terms fast and decisive. These issues emphasize the need for flexibility on the part of all parties in licensing terms with small startups.

D. Keys to Successful Engagement

In spite of these obstacles, multiple examples show that communication and collaboration can indeed be successfully and effectively carried out between industry and basic researchers. Several examples will be described below. What are the common characteristics that enable these successful interactions and collaborations?

A key characteristic required is trust. Particularly in collaborative efforts, the key to overcoming (1) basic researchers' concerns about excessive restrictions, and (2) industry's concerns about inappropriate disclosure of proprietary information, is developing a pattern of trust between individuals through a step-by-step process that establishes a track record. To promote such engagement between basic research and industry, leaders are needed who have experience spanning both basic research and industrial environments. Such individuals make a critical contribution by recognizing the sensitivities on both sides and helping to mediate them.

Early-stage basic research is sometimes considered "precompetitive" in the sense that information can be freely and publicly shared among different parties, including multiple industries. In many cases, however, it is in fact precisely in the early stages of the scientific understanding of a field that the broadest concepts emerge, leading to the broadest and most powerful patents. This is particularly true in less-mature technology areas. Therefore, in most cases of significant collaboration, proprietary information clauses in agreements are essential to enable meaningful discussions with participants. These clauses typically require a clear labeling of confidential information and prompt documentation of any ideas emerging in the verbal exchanges. However, to make this a workable process, such labeling must be limited to only the specific and truly confidential material rather than indiscriminately applied to all shared information.

The key to resolving IP issues is flexibility and compromise, as well as choosing appropriate topics for research. Industry and basic researchers should preferably find topics that will allow some, if not all, of the work to be published, perhaps after some delay for filing of patents, thus satisfying basic researchers' incentives for publication and public recognition. By the same token, basic researchers must agree to be sensitive to industry concerns about maintaining confidentiality on particular aspects of the work, and they should avoid situations in which they work simultaneously with competing companies on related topics.

One key to resolving licensing issues is for research institutions and commercial entities to moderate their expectations and demands with respect to upfront fees and royalties. All must recognize that energy technologies are complex and multifaceted, so that to develop a given technology, a company may license not just one, but a host of patents from multiple organizations. A high royalty, multiplied several times over, can easily lead to total royalty payments comparable to an industry's envisioned profit margin, thus undermining the commercial viability of the technology. At the same time, upfront fees are generally used to recoup costs of patenting and licensing — important to most research institutions in which technology transfer costs are not incorporated or otherwise paid for by research grants. Finally, it is important that research institutions continually bear in mind that the primary responsibility of their technology transfer activity is in the commercialization of inventions — and not in maximizing income from commercialization activities — and that therefore, they should set reasonable expectations regarding the value of IP. Without commercialization, IP has no inherent value.

Another important factor in building trust is to manage expectations as well as consistency. To this end, it might be desirable for the DOE and DOE Laboratories to be as consistent as possible in the terms and conditions for agreements executed with commercial partners, especially those that enter into several agreements over the course of time for similar technologies. Seemingly arbitrary changes to agreements can confuse and create mistrust. Another way to better manage expectations is to make a 'playbook' available that contain model agreements and licenses, as well as a 'what to expect' overview of the licensing and CRADA processes. Making available 'model' licenses that outline previously executed terms and conditions for various technologies can help make the negotiation process more efficient.

Industry's responsibilities in licensing negotiations are no less significant. Industry must accept reasonable license fees to the various licensors; the definition of "reasonable" will come from experience in negotiating a multiplicity of agreements, and any information that can be obtained about other license rates in the sector. Another key to resolving licensing issues is for industry to clearly differentiate where an exclusive license is really required, or where a non-exclusive license would suffice, since exclusive licenses are generally much harder to negotiate and more costly. With regard to the clause requiring products to be "substantially manufactured in the United States," national laboratory contractors may have to seek exemptions to this provision from DOE, which can significantly delay the license negotiations. Exemptions are allowed in cases where the license can be demonstrated to give substantial U.S. benefit. It is incumbent on licensor and licensee to work together in preparing a business case to communicate these benefits to DOE and trade representatives for approval. For clean-energy technologies, there may be benefits to the global environment and U.S. energy security that are added considerations to the case, in addition to the economic benefits that might accrue.

E. Modes of Engagement between Basic Research and Industry

There are many possible modes of engagement between industry and basic researchers, including collaborations that have been validated in programs sponsored by DOE, some through technology offices and some through BES. The following examples are not meant to be exclusive; new modes are likely to be developed in the future.

A certain amount of communication occurs at existing conferences. Indeed, the Basic Energy Sciences Advisory Committee (BESAC) Workshop on Science for Energy Technology was an important opportunity for communication between basic researchers and industry in a variety of clean energy fields. Future workshops or targeted meetings could highlight BES capabilities and activities, with invitations to key industrial leaders. Such meetings can start as being simply informational, but they could also be geared to investigating opportunities for meaningful collaboration, much as in the recent BESAC Workshop.

The recently established and BES-supported Energy Frontier Research Centers (EFRCs) and also the planned Innovation Hubs open a unique opportunity to establish communication and collaboration efforts with industry. Some of the EFRCs already include industry representatives, but BES could further encourage EFRCs to expand industrial collaborations and to identify and address the science issues industry faces. Given the substantial $125-million-per-year scope of this program, these centers could provide a major vehicle for encouraging such engagement. The EFRCs themselves can run workshops that seek to involve industry. Sometimes, where IP issues are not so sensitive, collaborative programs can be based simply on informal communication, provision of samples, and sharing of results.

Cooperative Research and Development Agreements (CRADAs) are partnerships in which a private sector partner and a national laboratory work together on research and development. In the simplest form of a CRADA partnership, each party contributes equally to the project. In more complex arrangements, the private partner may opt for a “funds in” arrangement, in which it supports part of the laboratory's expenses. When work is complete, each party retains title to its own inventions or intellectual property. In addition, commercially valuable information developed under a CRADA may be protected from disclosure for up to five years. One issue for CRADA funding is that national laboratories typically have limited non-federal discretionary funding to support CRADA activity. One potential solution would be for DOE to allow national laboratories to use laboratory-directed research and development (LDRD) funds for this purpose.

BES-supported researchers interacting with industry can benefit by any of the above models, but other steps that could be taken to enhance interactions include the following:

- BES could develop a more robust industry-outreach program. Information on a website is a first step, but increased communication directed to specific industries could be more effective. As mentioned above, workshops or targeted meetings could highlight BES capabilities and activities, with invitations to key industrial leaders, ideally including not just industrial researchers but also individuals at the chief technical officer or department head level.

- Communication of industrial perspectives and needs to the BES research community is equally important. Internal seminars inviting industrial speakers and internal discussions about how BES capabilities could be brought to bear on industrial needs could be encouraged.

- As discussed in Chapter 11, the BES-supported user facilities can play a special role in facilitating industrial research and in stimulating collaborative efforts.

- DOE might consider whether the national laboratories could engage in cooperative research with industry with the use of LDRD funds toward a laboratory's share of CRADA work.

- DOE and the DOE Laboratories should consider whether licenses and CRADA agreements could be made more consistent across different labs, as well as making a 'playbook' with model agreements readily available to potential research partners and licensees.

- BES could consider strategies to engage industry sectors broadly, for example, by working with industry in consortia. Such consortia could identify the common science issues faced by a large segment of industry and communicate them effectively to BES and other basic science organizations.

- BES should consider funding "dream teams" drawn from the ranks of outstanding scientists in both basic research and industrial communities to pursue the basic science solutions behind performance-limiting roadblocks to industrial development of clean-energy technologies. The challenges that such grants might support could include, but would not be limited to, the priority research directions identified in this report.

F. Examples of Engagement Between Basic Scientists and Industry

The following examples illustrate possible approaches and principles for engagement of basic scientists with industry that have been used successfully in the past. It should be understood that many other modes of interaction have been used, and flexibility is always required to address the particularities of each given situation.

1. The Wire Development Group

The Wire Development Group is a collaboration that includes one company, American Superconductor Corporation (AMSC), and researchers from multiple national laboratories and universities that has been addressing materials science underlying high-temperature superconductor (HTS) wires through active, day-to-day collaboration between industry and basic researchers. The agreements between AMSC and the national laboratories are CRADAs, supported 50–50 by AMSC and DOE's Office of Energy Efficiency and Renewable Energy (EERE) and Office of Electricity Delivery and Energy Reliability (OE). This unique collaborative effort has persisted now for almost two decades, aiding AMSC in developing HTS wire and positioning the United States to lead in the introduction and deployment of a major new energy technology.

The research of the Wire Development Group deals with proprietary issues related to the current carrying capability and cost of superconducting wire and is specific to American Superconductor's manufacturing process, precluding the participation of other companies in the collaboration. This collaboration differs from a multi-company consortium for developing low-temperature superconductor wire in the 1980s for DOE high-energy physics projects. In that case, DOE was itself the dominant partner and customer, and the role of proprietary information and inter-company competition was much less prominent.

A multiparty proprietary information agreement (PIA) signed by all parties in the Wire Development Group protects information – including proprietary AMSC information – disclosed in the course of the regular participant meetings, enabling free and active discussion and direct joint involvement in the research. It was a challenge to reach common agreement on the PIA's legal language among three such diverse parties — industry, university, and national laboratory operators; the key was getting the legal and technology transfer officers to understand the clear ground rules and scope of the collaboration. Over time, all parties have come to appreciate industry's need for confidentiality and basic researchers' need for rapid, high impact publication. These issues need to be addressed on a case by case basis. Access to AMSC's state-of-the-art materials, as well as to the insights of its research and development (R&D) team, has been a major motivator to the basic researchers, while AMSC has benefited from the engagement of top-notch scientists with state-of-the-art analytical and experimental capabilities at the national laboratories and universities.

2. Semiconductor Research Corporation (SRC)

The Semiconductor Research Corporation (SRC) is another successful model for industry–university engagement. Formed in 1982 by a group of visionary leaders from competing semiconductor companies, SRC is a nonprofit industry consortium that invests in basic university research addressing a broad range of industry needs. Since its inception, SRC's objectives have been to support the competitiveness of its members, explore new technologies, stimulate industry-relevant academic research, promote greater collaboration within academia, and generate a pool of experienced faculty and relevantly educated students.

SRC has had a substantial impact on both the industry and the university research community. Through a total investment of over $1.5 billion, SRC has created a substantial academic research enterprise, funding nearly 2000 faculty at over 240 universities around the world. SRC-funded research comprises a significant fraction (~20%) of the annual scientific literature related to silicon-based technologies. Materials, design tools, and processes based on SRC research are widely used across the industry. By funding pre-competitive research and sharing the results with all members, the impact of SRC's investment has been greater than a similar investment made by the companies individually would have been.

In the course of funding university research, SRC has supported over 8000 students, most of whom remain in the semiconductor community. SRC students benefit from working on industry-relevant research problems and receiving mentoring and other meaningful industry contacts as part of their education. As a result, they are extremely well-prepared and able to "hit the ground running" when they begin their careers, whether in industry, national laboratories, or academia.

Finally, SRC has developed processes to maximize the effectiveness and efficiency of its research. These include processes to identify technological barriers and research priorities, to provide input and feedback during the research, and to deliver research results to member companies in near-real time. In-person reviews and other events ensure that SRC-funded faculty and students build relationships with other academics working in the field and with industry experts. These connections have long-lasting benefits for both sides — allowing university researchers to be more informed about industry needs and facilitating technology transfer and awareness of cutting-edge science within industry. However, the research typically is carried out by faculty and students without any inventive contribution by industry. Under the terms of SRC's research contracts, ownership of any resulting IP remains with the university and SRC retains a nonexclusive license for use by its member companies. Some aspects of SRC are associated particularly with the semiconductor industry, such as the drive of the entire industry to maintain the pace of scaling to smaller dimensions described by Moore's Law. Nevertheless, the SRC model could be considered in other industries where there are mutually defined basic research needs for which consortium members are willing to waive exclusivity. Recently, SRC has launched an Energy Research Initiative with a diverse set of member companies to conduct fundamental research on photovoltaic and smart grid technologies.

3. Sandia Combustion Research Facility

The Combustion Research Facility (CRF) at Sandia National Laboratories-California is a unique center for integrating basic and applied research in combustion science and technology. BES operates the CRF as a collaborative laboratory that attracts visiting scientists from academia, national laboratories, and industry from around the world. CRF supports vigorous, in-house fundamental research on combustion chemistry, advanced laser diagnostics, and state-of-the-art combustion simulation. The EERE Vehicle Technologies Program supports a complementary program on internal combustion engine technology. This, in turn, feeds directly into a wide range of collaborations with industry and industry-supported programs. Examples of the transfer of knowledge between the BES and EERE programs and on to industry are numerous over the CRF's 28-year history, and include the recent achievement of a major milestone in industrial engine design — the first all-computationally designed diesel engine by Cummins Inc., based on science developed at CRF.

The key to the successful collaboration of industry with CRF is a Memorandum of Understanding (MOU) defining a specific precompetitive space for CRF's work on the science underlying combustion, while industry focuses on engine design. Because of the relative maturity of the combustion field, participating engine manufacturers and energy suppliers urged CRF to minimize patenting and to publish results in peer-reviewed journals after prior industry review. Another key to minimizing competitive issues is that although guided by industry, the work is largely carried out by national laboratory personnel without day-by-day industrial research involvement. All results are then available to all industry participants, without compromising any one company's intellectual property. This model is a subset of that established by the United States Council for Automotive Research (USCAR) consortium, which also defines precompetitive research topics in fields such as batteries and lightweight structures.

Examples of precompetitive research at the CRF include the development and application of laser diagnostics for reacting flows and the creation of high-fidelity computational combustion modeling supported by BES, which, when combined with the application of these tools supported by EERE, were key enablers for designing the aforementioned Cummins engine. Figure 2-2 illustrates a flame simulation of the complex turbulent flows and chemistry typically found in combustion.

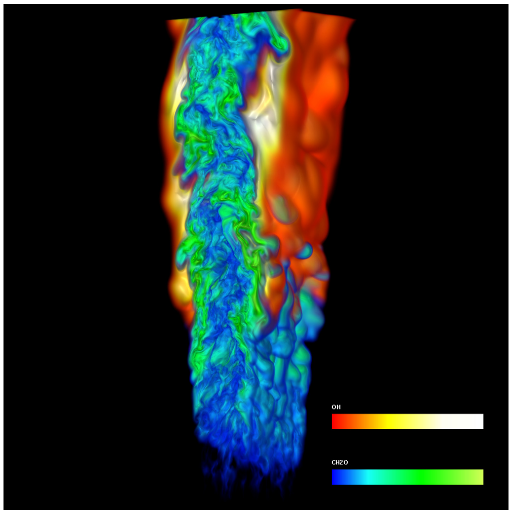


Figure 2-2 This state-of-the-art flame simulation, developed under BES funding, provides fundamental insight into turbulence-chemistry interactions towards the development of the next generation of computational models to be used in clean and efficient internal combustion engine design. Source: J. Chen, C.-S. Yoo and H. Yu, Sandia National Laboratories.

4. Brookhaven National Laboratory CRADA

CRADAs are a major vehicle for advancing collaborations between basic researchers and industry. One example is work at BNL on advancing the commercial potential of low-temperature fuel cells for automotive and stationary applications. Barriers to widespread commercialization of fuel cells have been significantly reduced by demonstrated key improvements in cost and reliability of critical electrocatalyst materials. BES initiated a basic research project at BNL in 1992, centered on fundamental studies of electrochemical interface structure and properties. These studies led to the realization that the electrochemical activity of metals could be tuned by putting a single atomic layer of one metal over another. This in turn led to the synthesis of tailored core-shell nanoparticles, with one or two layers of atoms of one active metal decorating a core particle comprised of a second metal. These core-shell nano-catalysts were further developed under funding by the fuel cell program in EERE in the period 2003-2010. The coordinated BES and EERE research has resulted in electrocatalysts for fuel cells that demonstrate a 4- to 20-fold reduction in the amount of expensive platinum necessary for good performance and show important improvements in long-term stability. A strong basic understanding and breakthrough synthesis methods developed under BES funding, along with key characterization at two BES user facilities at BNL, the National Synchrotron Light Source and the Center for Functional Nanomaterials, were critical to the development of these novel nano-catalysts for fuel cells. This research program has so far generated 7 issued U.S. patents, 9 pending non-provisional U.S. patent applications, and 2 pending provisional U.S. patent applications which are owned by BNL and cover many key aspects of fuel cell electrocatalysts.

Based on these promising results and starting in 2005, BNL entered into Cooperative Research and Development Agreements funded by industrial partners (GM, Toyota, UTC Fuel Cells, Battelle) and this work has furthered the commercial potential by scaling up the synthetic methods. Now commercial partners believe that these core-shell nano-catalysts are currently the most promising electrocatalyst path for commercialization of low-temperature fuel cells for automotive and stationary applications. The BNL intellectual property portfolio has been an important factor in attracting CRADA and commercialization partners, providing them opportunities for a competitive market position through licensing. The CRADA mechanism is one key to developing a long-term relationship with commercial parties, as well as providing researchers at DOE Laboratories an invaluable "window" on real-world deployment and commercialization barriers. Brookhaven Science Associates' (BSA) Technology Maturation Program provided funding to advance the technological readiness for laboratory inventions, including scale-up or life-cycle demonstrations/testing, in order to improve commercial potential. In this case, the BSA Technology Maturation funding supported the scale-up of the synthesis from test quantities (milligrams or less) to 10-gram batches and the development of an in-house membrane electrolyte assembly (MEA) fabrication and Fuel Cell Test Station for testing larger scale assembled fuel cells. This scale-up effort has proved to be a key to moving the technology along the path from the laboratory to deployment.

G. Workforce Development

Workforce availability is another important barrier to progress in development of clean-energy technology. Creating a workforce conversant in basic science and clean-energy technology that can meet our energy and economic challenges is a major task. Universities must play a leading role in providing curriculum and guidance for the next generation of energy scientists and engineers. BES can play a key role in developing the workforce by implementing some of the mechanisms for greater communication and collaboration outlined in this report. Workshops, staff exchange grants across the basic science–industry interface, and collaborative research, will promote cross-training of the existing and next generations of energy researchers, strengthening the ties between industry and basic science. Industry can make major contributions by establishing fellowships, co-funding university research programs, participating in cooperative programs, providing tuition support, sponsoring conferences and job fairs, and conducting its own internal training. With the prospect of rapid growth in the clean-energy technology industry, the scope of such programs could be further expanded.

In addition to funding research and fellowships that will attract faculty and students, BES can take steps to increase the flow of students into careers in the basic science of clean-energy technology. The newly established DOE Office of Science graduate student fellowships will help attract top-notch students to the energy field. The basic energy science–industry interaction grants could support student internships and cooperatives in industry. Such experiences provide an excellent introduction to industrial careers in science and engineering, and would establish continuing university–industry relationships that would encourage further interactions.

The talent pool created by BES support of the research priorities and interaction opportunities identified in this report will drive technological innovation based on basic science that can create future clean technology products and jobs, as well as new companies.

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Chapter 3: Panel 1 — Solar Electricity from Photovoltaics
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I. EXECUTIVE SUMMARY

The widespread penetration of photovoltaic solar electricity requires significant advances in higher performance, lower cost, and increased reliability to compete effectively against fossil fuel alternatives. Three science areas are identified as critical: fundamental properties of photovoltaic interfaces, advanced photovoltaic analysis and computational modeling for scale-up, and better control of photovoltaic lifetime and degradation processes. Advances in these areas will enable established photovoltaic technologies to break through the economic barrier to widespread adoption, with transformative impact for renewable solar energy as a major contributor to electrical energy supply.

II. PANEL REPORT

Role of Solar Photovoltaics in the National Energy Picture

Sunlight is the largest potential source of carbon-free electricity. More energy from the sun hits the surface of the earth in one hour than that currently consumed by humans in a year [1,2]. As an established source of renewable electricity, photovoltaics have the potential to supply a significant fraction of our national electricity needs [3].

Factors that help photovoltaics compete with other electricity generation include:

- Photovoltaics produce electricity during the day, when rates are highest and demand is strongest;
- Photovoltaics produce no carbon emissions, no noxious gases such as oxides of nitrogen or sulfur, and no particulate emissions;
- Photovoltaics have no exposure to fuel price volatility;

- Photovoltaics can last at least 30 years, and potentially a hundred years, if designed for that duration;
- Photovoltaics operate simply, and most systems do not need elaborate on-site monitoring;
- Photovoltaic operating cost, once capital investment is paid off, is about 1 ¢/kWh; and
- Photovoltaics reduce homeowner electricity bills, hedge against fluctuations in energy prices, and avoid high retail rates in some locations [4] (e.g., over 20 ¢/kWh in Hawaii, Massachusetts, and Long Island).

The initial cost of photovoltaics remains the biggest barrier to their broad use as reduced carbon energy sources and as buffers against fossil fuel price escalations. Incentives defray part of the high installation cost of carbon-free energy sources, and photovoltaics join wind, solar thermal electric, nuclear, wave, and geothermal electricity in this market. But to achieve transformative impact, photovoltaics must compete effectively without a subsidy on a commercial basis. Low cost is the critical element: $1/watt is seen as a target level enabling broad cost-effective competition with fossil energy.

Progress in photovoltaic research and development has achieved a well-documented reduction of about 97% of the original prices in the 1970s (Fig. 3-1). Research-driven pathways can be found that will yield a further 50% to 75% reduction with existing, commercial photovoltaic

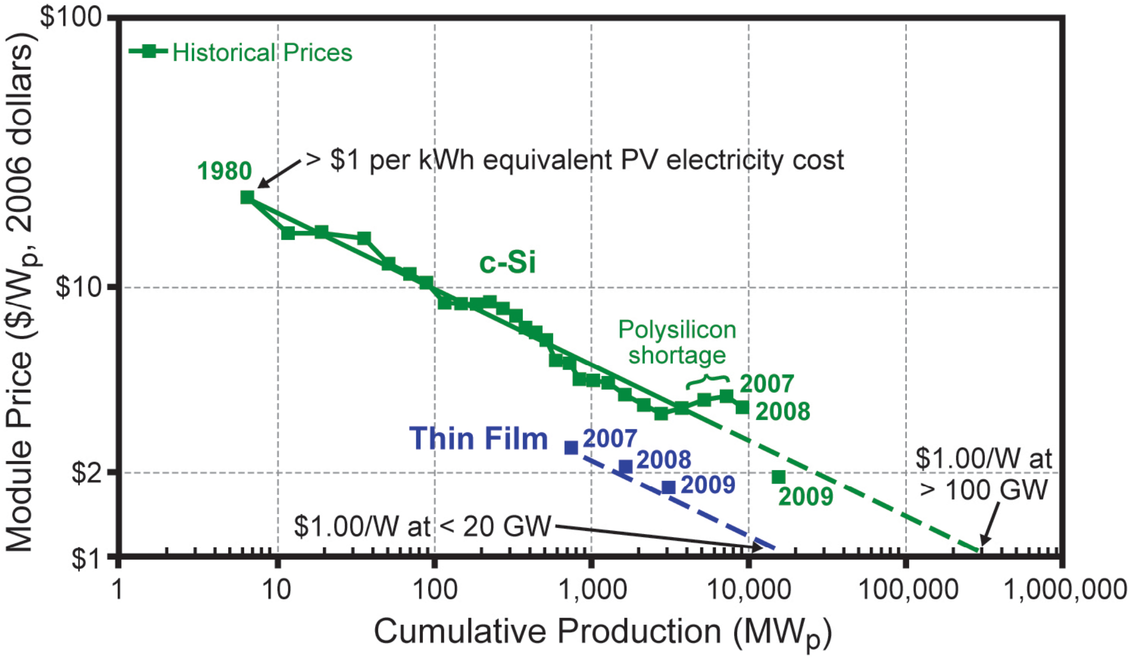

Figure 3-1 Photovoltaic price reduction has followed a steady, approximately 20% reduction for each doubling in production for silicon-based modules (green curve). During 2004-2008, an imbalance in supply and demand led to temporarily higher prices that have now re-equilibrated with the historical curve. A cost of $1/watt is seen as a target level enabling broad cost-effective competition with fossil energy. Source: National Renewable Energy Laboratory.

technologies [5]. At such price levels, photovoltaics would be competitive with any other carbon-free electricity source.

For the near term, photovoltaics can be integrated with our electricity grid without the need for major infrastructure changes. Advances in solar forecasting will help to anticipate and accommodate intermittent photovoltaic generation, as wind forecasting helps to accommodate variable wind generation. Studies suggest that as much as 20% of our electricity could come from intermittent sources before we would need more radical grid modifications such as storage [6]. Trends toward a more integrated "smart" grid will help clear the way for greater responsiveness and greater capacity for renewable sources.

Status of Present and Ultimate Potential for Photovoltaics

Figure 3-2 shows the adoption of nuclear, wind, and natural gas turbines, and the parallel path of recent photovoltaic deployment. About 22 gigawatts (GW) of solar photovoltaics have been deployed worldwide as of early 2010, including 7.2 GW deployed in 2009 [7]. This is equivalent to about five 1000-megawatt (MW) baseload power plants worldwide, since about 4 GW of photovoltaics produce about the same number of kilowatt-hours (kWh) as one GW of baseload power.

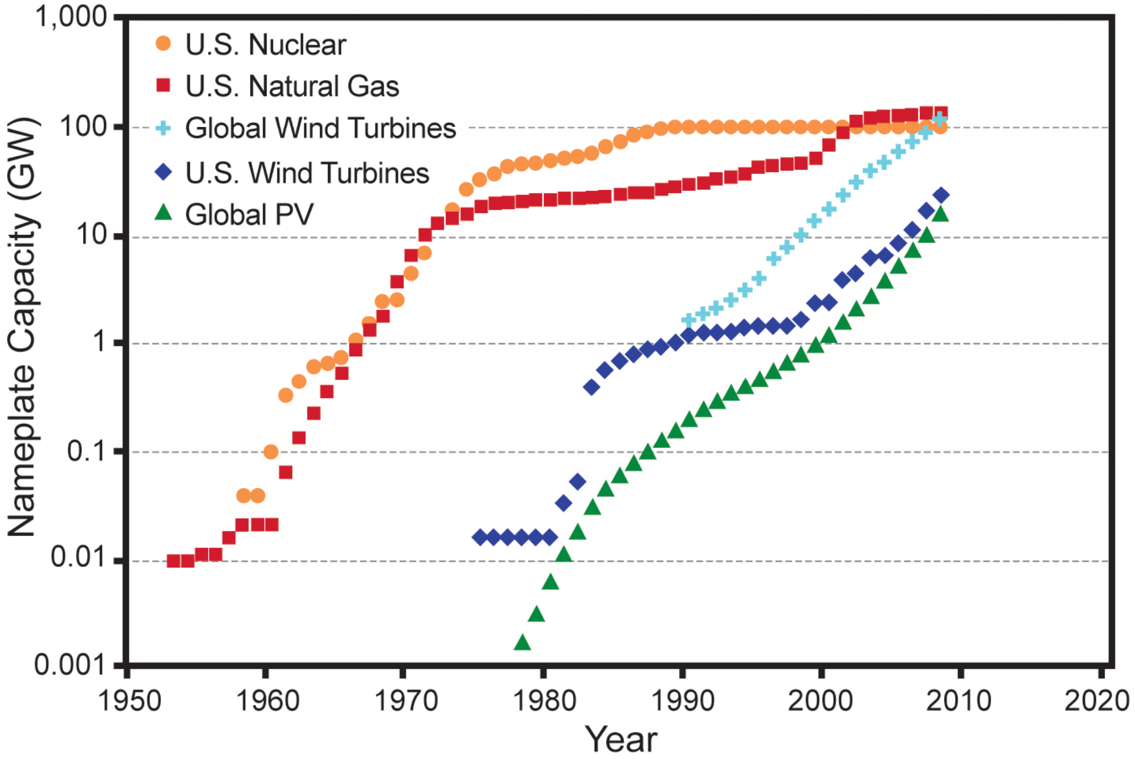

Figure 3-2 Nuclear, natural gas turbines, and wind turbines have been rapidly adopted by the energy industry and, to date, photovoltaics are on a parallel path. Source: International Energy Agency.

Annual photovoltaic installations in the last decade grew at about 50% per year. In 2009, the growth rate was lower (about 20%), influenced by the global recession.

The U.S. presence in photovoltaics is small on a scale relative to our energy use. The United States accounts for one-fifth of world energy use, but only one-tenth of world photovoltaic installations. The United States has about 2 GW of photovoltaics deployed, with 0.5 GW of new photovoltaics added in 2009 [8]. Similarly, the United States has a smaller manufacturing base in photovoltaics than other nations, which have been more aggressive in deploying low carbon technologies.

The U.S. status in terms of technical leadership in photovoltaics is much higher. U.S.-owned companies are at the forefront of several of the key technology options (Table 3-1). This is partly the result of an effective Department of Energy solar development program in place since the late 1970s.

Roadmaps for halving today's photovoltaic costs have been published by technical agencies and by leading photovoltaic companies. A cost of \$1–2 per watt (W) for a fully installed system appears achievable, making photovoltaics fully competitive with other low-carbon electricity sources — wind, nuclear, solar thermal electric — and with the expected cost of carbon-sequestered coal electricity.

Table 3-1 Photovoltaic Technologies and U. S. Corporate Leaders

Technology	Company (U.S. Leadership)	Comment
Mono-crystalline silicon	SunPower	Ultra-high efficiency modules and low-cost trackers
Polycrystalline silicon		Dominated by China
Cadmium telluride	First Solar	World's largest photovoltaic module manufacturer; lowest cost photovoltaic technology (<\$1/W)
Copper indium selenide alloys	Several contenders	Emerging technology with no clear leader
Thin film amorphous and microcrystalline silicon alloys	UniSolar (ECD) and Applied Materials	Lead shared with Japan and Europe
III-V multijunctions for concentrators	Spectrolab and Emcore	Direct descendant of U.S. space program
Concentrator photovoltaic	Amonix and SolFocus	Emerging technology with no clear leader
Organic photovoltaic	Konarka, Plextronics, Solarmer	Emerging technology

Approximately 600 GW of photovoltaic capacity could be installed on roofs in the United States, roughly half on commercial buildings and half on residences. This could provide about 400 terawatt hours per year (TWh/yr) of electricity, or 10% of our current demand. There is no similar limit on ground-based systems. It would take about 0.7% of U.S. land area covered with photovoltaic cells at an efficiency of 10% to meet the electricity needs of the entire United States [9,10].

The installed cost per watt of large photovoltaic systems is about 25% lower than that of small ones [11]. Similarly, the output of photovoltaics (PVs) in the sunnier southwestern United States is about 50% higher than the output in average locations. Thus, large systems in the southwest are two to three times less expensive per kWh than residential systems on the east coast, making them attractive opportunities for utility-scale development.

Several studies have examined the supply chain and labor challenges inherent in rapidly reaching multi-TW scale with photovoltaics [12]. These issues include short-term supply bottlenecks such as a mismatch in supply and demand, and the challenge of availability of elements such as tellurium, indium, selenium, and gallium used in thin film technologies. For example, the need for tellurium, one of the most sensitive materials, can be reduced from over 100 metric tons per GW to about 13 metric tons per GW by increasing module efficiency from 10% to 15% and thinning layers of cadmium telluride from 3 microns to 2/3 of a micron. With these improvements, maximum annual cadmium telluride module production from currently identified ores (about 1500 metric tons per year of tellurium as a by-product of copper) could increase to about 150 GW per year (GW/yr) [13].

Established photovoltaic technologies — mono-crystalline silicon, polycrystalline silicon, cadmium telluride thin film, and amorphous silicon — can meet the desired strategic level of deployment in the United States and globally. But many research challenges must be overcome to drive the performance, cost, and reliability of photovoltaics to levels that are cost-effectively competitive with fossil energy. Key challenges include thinning the active material layer to lower the materials cost, decreasing defects and recombination centers at interfaces to improve efficiencies, and designing new protective materials for longer-term stability. In addition to the established photovoltaic technologies, there are a host of research challenges in emerging technologies such as organic photovoltaics, copper indium selenide alloy thin films, concentrating photovoltaics, and dye-sensitized photovoltaics; as well as in laboratory research areas like quantum dot, intermediate band, and hot carrier photovoltaics. Scientific challenges include understanding fundamental parameters such as carrier lifetime, recombination velocities, and degradation mechanisms. Additionally, future technologies should employ materials that use green processing, earth-abundant elements, and low-cost manufacturing.

Context and Background for the Priority Research Directions (PRDs)

Except for crystalline silicon where research has powered Moore's law progress over decades, the leading photovoltaic technologies lack a strong scientific foundation, and progress, successful as it is (Fig. 3-3), is largely empirically driven. Advances are needed in all aspects of photovoltaics: materials, interfaces, processes for making and altering photovoltaic devices, advanced photovoltaic device layers, and scale-up from small to square meter devices and then to square miles of annual output at high yield. Melded with these challenges are aspects of device efficiency, device stability, and process stability. The PRDs presented here provide the needed scientific understanding. They overlap with those of the earlier Basic Research Needs (BRN) workshop on solar energy, April 18–21, 2005 [2]. However, the present focus is more on building scientific understanding of *existing* photovoltaic systems rather than on the discovery and exploration of completely new and revolutionary materials and approaches. Both areas are critical, but the Workshop panel focused on existing materials to open a path to nearer term impact, commercial deployment and U.S. competitiveness.

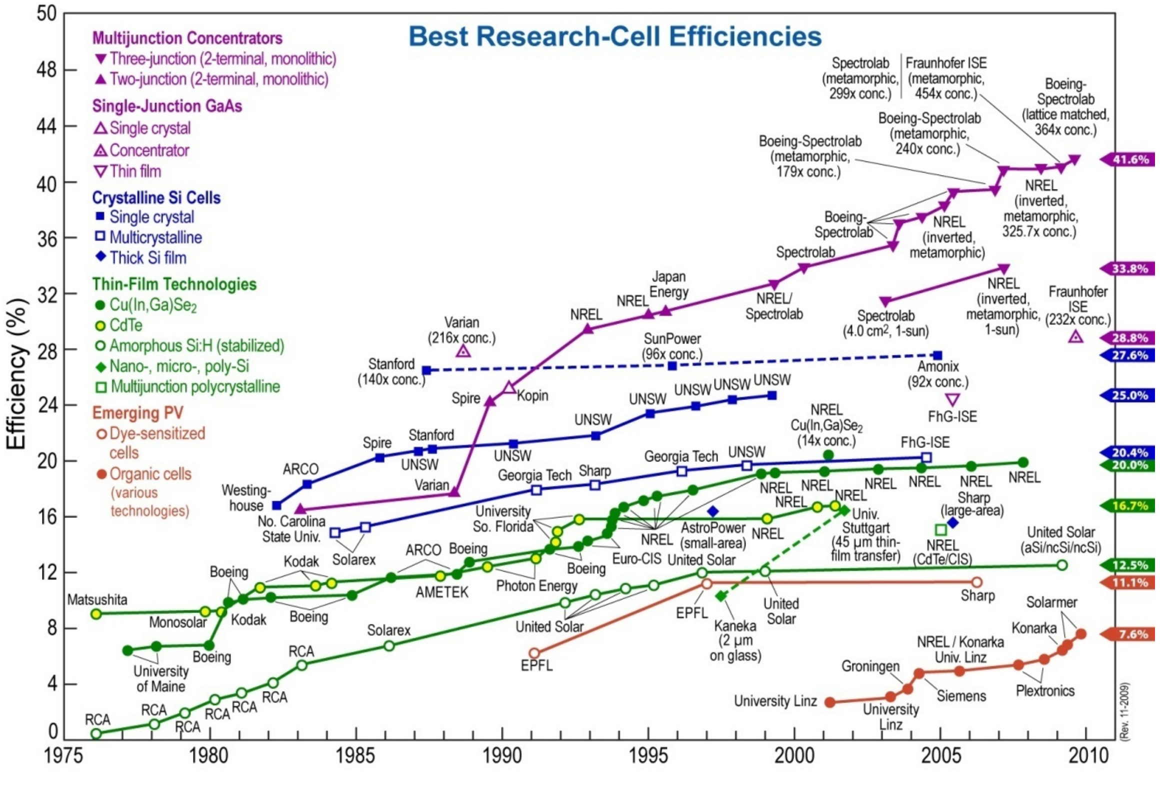

Figure 3-3 Progress in cell efficiency is core to progress in commercial penetration, since it defines technologies worthy of scaling up and promising pathways ripe for further module and system cost reduction. This progress has been steady and successful, but based on empirical approaches rather than on fundamental materials and device science. Source: National Renewable Energy Laboratory.

Brief Description of Priority Research Directions

PRD #1. Fundamental Properties of Photovoltaic Interfaces

Many of the most critical issues of photovoltaic device performance and reliability occur at interfaces such as p-n junctions, the back and front device contacts, light and carrier reflectors, tunnel junctions, passivation and buffer layers, grain boundaries in polycrystalline semiconductors, or encapsulants and packaging materials (see Fig. 3-4).

Examples of needed research include: prediction and evaluation of interface intermixing; improvement of contact resistance to high work-function, high resistance materials such as cadmium telluride; better understanding of the physics, chemistry, and stability of grain boundaries in polycrystalline semiconductors; and improvement of the adherence and lifetime of semiconductor or metal/encapsulant and packaging interfaces. Considering the issues above, there is a strong need for fundamental insights into interfaces of photovoltaic cells and modules. While most work to date has been empirical, there is an opportunity to use more sophisticated tools and expertise to better understand the optical, electrical, mechanical, and chemical interface properties, and to predict and ultimately to control their changes.

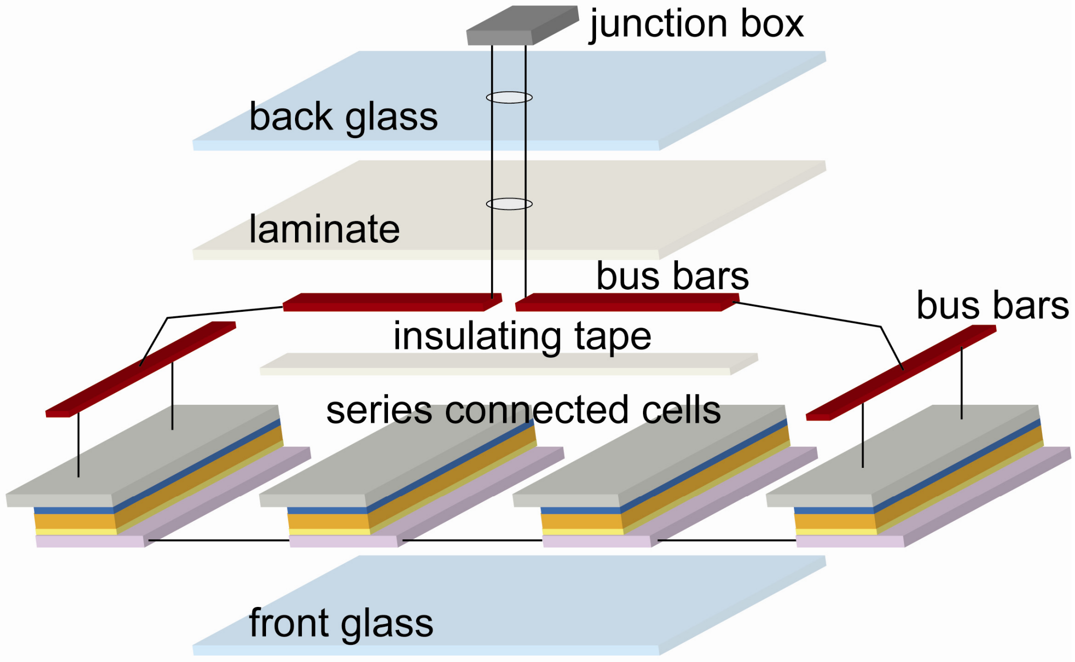

Figure 3-4 Exploded view of a thin film module. The series-connected cells include the front transparent conductive oxide, absorber, and back reflector. Light enters the module from the bottom.

PRD #2. Advanced Photovoltaic Analysis and Computational Modeling for Scale-up

Computational models and tools are needed to help correlate processing parameters with fundamental device physics to accelerate research and commercial photovoltaic product development. Within existing silicon and thin film-based modules, one such opportunity is to explore materials parameter space for optimizing electronic and optical properties. Understanding complex inter-relationships between materials properties, process parameters, and ultimate performance will benefit not just device performance, but also development of in situ process controls and in-line diagnostics for improved manufacturing yield for very large area high-throughput processes. Overcoming these challenges requires sophisticated new modeling tools coupled to advanced and insightful analysis.

PRD #3. Photovoltaic Module Lifetime and Degradation Science

An improved understanding of degradation mechanisms and development of specific new protective materials would increase module lifetimes and lower the cost of photovoltaics. We have a limited grasp of photochemical degradation, dielectric degradation, and leakage current in the presence of water and oxygen. Equally lacking is an understanding of long-term impurity diffusion processes that occur in semiconductors and through interfaces, especially in large-area devices that have inevitable compositional variations in all dimensions. In addition, we need well-designed accelerated stress tests to define and evaluate potential degradation mechanisms, parallel accelerated lifetime models, and the incorporation of mechanistic degradation rates that correlate data with actual outdoor performance over many decades.

III. PRIORITY RESEARCH DIRECTIONS

A. PRD #1. Fundamental Properties of Photovoltaic Interfaces

1. Problem Statement

Deeper understanding of interface behavior is critical for efficiency enhancement, yield optimization, reliability improvement, cost reduction, and ultimately, broad penetration of photovoltaic products. While most work to date has been empirical, more sophisticated tools and expertise could improve our understanding of optical, electrical, mechanical, and chemical interface properties, and allow prediction of their changes over time. Fundamental knowledge of interface variability spanning device and package construction is also needed.

2. Executive Summary

The development of a deep scientific understanding of the physics, chemistry, and materials properties relevant to the degradation of interfaces will result in high-performing, high-yielding fabrication processes and improved competitiveness of the photovoltaic industry. The industry need is for progress in theory and advanced characterization of photovoltaic interfaces, in order to greatly accelerate the application of new materials and processes and decrease the gap between laboratory/pilot line and full-scale production. Research directions include studying the interfaces of advanced heterogeneous materials, the time-dependent behavior of interface traps, and effect of random interface morphological defects on electro-optic behavior. The ultimate impact would be to facilitate the development of more efficient, reproducible, reliable, and inexpensive photovoltaic products for broad harnessing of solar energy.

3. Industry Need

The photovoltaic industry is currently undergoing massive scale-up driving new requirements for performance, yield, process control, and reliability. Meeting these needs requires rigorous understanding of interfaces between materials. Crystalline silicon and thin film amorphous silicon have been studied empirically and perfected for several decades, providing a wealth of information to guide development and validation of the scientific understanding of performance, yield, and process control, which would immediately raise productivity and lower cost. New process steps are being introduced to photovoltaic technologies, requiring an equivalent scientific understanding and foundational approach. Examples include novel doping/metal pastes, advanced laser processes, new grades of starting material such as metallurgical-grade silicon, and new encapsulation materials and strategies. Promising new materials and processes also need evaluation in the context of implementation into field-capable products. This requires thorough understanding and analysis not only of the basic device building blocks, but also the impact of interfacial connections to other components of a completed module.

4. Scientific Challenges

The scientific challenges are broad, given the diversity of approaches currently undertaken by the photovoltaic industry. For thin-film photovoltaics, there are still many gaps in the understanding of deposition techniques, such as the link connecting equipment configuration and process conditions to material and interface quality, and ultimately, to process uniformity. Transparent conductive oxides and their possible replacements face fundamental questions regarding the best morphology and how to achieve it, as well as the impact of process choices on defect levels, light trapping, and electrical transport. For polycrystalline-silicon, a full description of the material, the trapping mechanism, and the impact of contamination is still lacking; and the impact of grain boundaries on performance and reliability is still not fully understood. Finally, for crystalline-silicon, the processing or firing of advanced metal pastes would benefit from a fundamental study of the constituent processes such as diffusion, strain, and trap creation.

5. Research Directions

- *Fundamental Characterization and Modeling of Interfacial Processes.* As high-efficiency crystalline-silicon cell designs increasingly incorporate high-precision interfacial patterns such as interdigitated features, it is imperative that the fundamental characteristics of metallic and dopant diffusion at interfaces for advanced printed pastes and for laser-created lithographic features are understood. Important interface characterization techniques include temperature-dependent capacitance-voltage, ultraviolet photoemission spectroscopy, and analytical transmission electron microscopy for determining trap densities and recombination velocities, the band alignments at the interface, and interfacial structural and chemical information, respectively. For example, synchrotron-based ultraviolet photoemission at U.S. Department of Energy (DOE) Office of Basic Energy Science (BES)-funded user facilities (Chapter 11) could be used to study metal-induced gap states and the effect of dopants on the band diagram in a crystalline-silicon cell that uses advanced pastes. These parameters are integral to the development of accurate optical-electrical models of interfaces in a device.

- *Prediction and evaluation of interface intermixing and diffusion in compound semiconductors* such as cadmium sulfide and cadmium telluride or copper-indium-gallium diselenide (CIGS) and organic photovoltaics. Surface analysis methods such as Auger electron spectroscopy and X-ray photoelectron spectroscopy depth profiles can show elemental diffusion across interfaces between sulfur (from cadmium sulfide) to the cadmium telluride or CIGS film, and secondary ion mass spectrometry (SIMS) can be used to profile the major constituents and impurities such as oxygen, carbon, and sodium. Time-of-flight SIMS (TOF-SIMS) has a high mass resolution, gives specific molecular information, and is therefore very useful for studying organics.

- *Better understanding of the physics, chemistry, and stability of crystalline defects and grain boundaries in polycrystalline semiconductors,* including highly compensated semiconductors such as upgraded metallurgical grade silicon. Phases and materials structure can be studied using X-ray diffraction, transmission electron microscopy, scanning electron microscopy, and atomic force microscopy. Nanoscale interfacial defects and elemental composition can be studied simultaneously with scanning transmission electron microscopy with analytical capabilities such as energy dispersive X-ray spectroscopy. For example, an energy dispersive X-ray spectroscopy line scan across a zinc oxide/cadmium sulfide/CIGS cell shows the elemental composition across different interfaces (Fig. 3-5).

- *Improvement of contact resistance to high-work function, high-resistance p-type material such as cadmium telluride.* Proprietary thin film recipes dominate this sector of the industry. At present, there is an inadequate scientific foundation to make fundamental advances and achieve optimal efficiencies.

- *Better understanding of the influence of randomly distributed interface inhomogeneities on device parameters.* For example, the interface between substrate and the intrinsic layer in silicon heterojunction cells is critical for device performance, which needs to be correlated with effects caused by defects, microstructure, and interfacial intermixing. This can be achieved by using the interface characterization techniques described above on a variety of tested and controlled devices. Three-dimensional modeling can help integrate and interpret these experimental results.

6. Potential Impact

Understanding and controlling interfaces in photovoltaic devices will promote industry growth through reduced production costs, a tighter distribution in module performance, predictability of performance, yield and field behavior, speed of adoption of new process modules, development of recognized models shared among academia and industry, and development of a workforce with deep technical knowledge in the photovoltaic field. The ultimate impact is to bring photovoltaic performance, cost, and reliability to a point of cost-effective competitiveness with fossil energy, unleashing a transformative growth of renewable solar energy sources for the world economy.

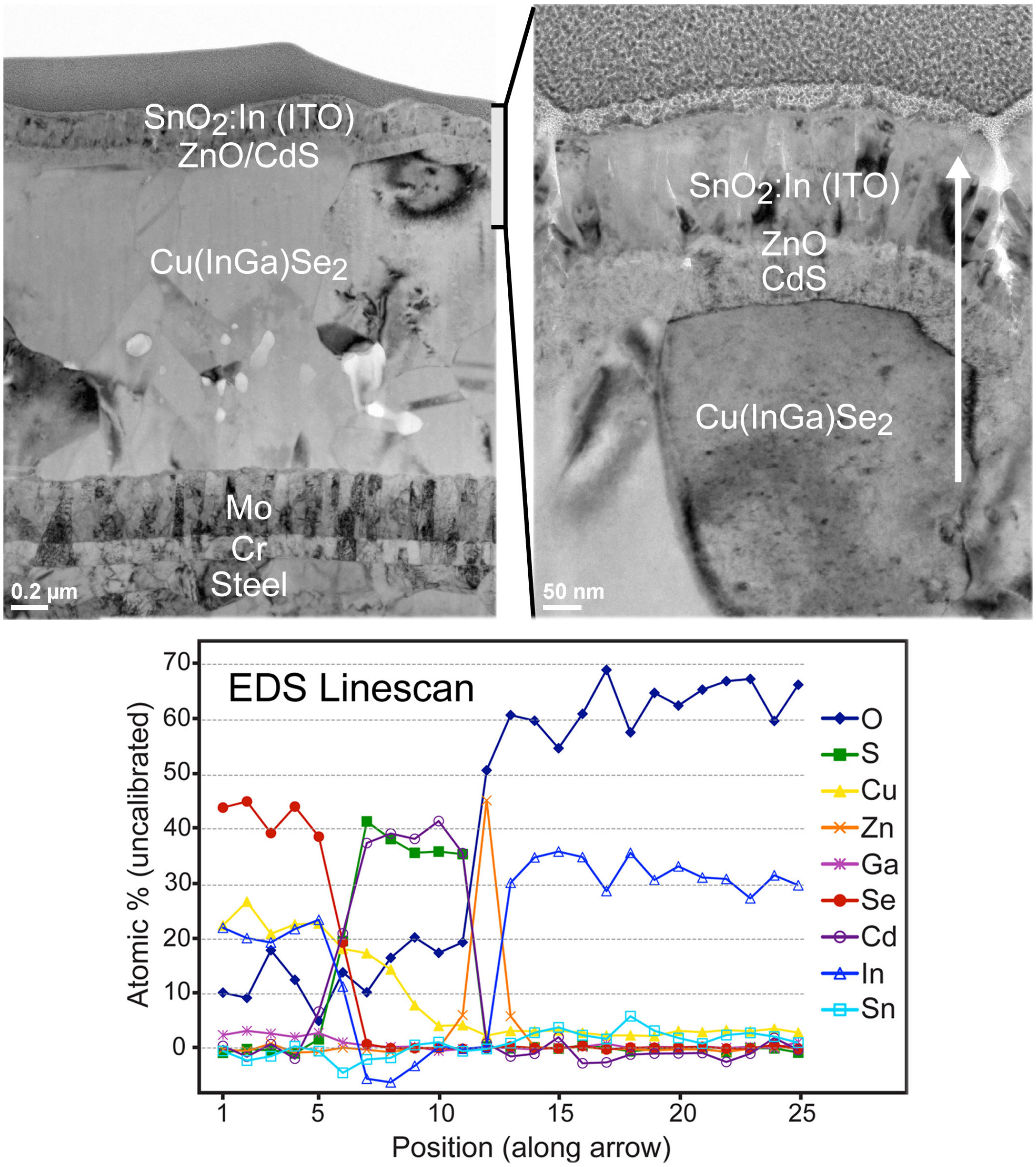

Figure 3-5 High-resolution cross-sectional transmission electron microscopy (TEM) images of a CIGS cell showing the grain boundaries and internal defects within the cell as well as the many active interfaces. An **energy-dispersive X-ray spectroscopy** (EDS) line-scan analysis (graph) gives the elemental profile across multiple interfaces. Arrow indicates location of linescan. Source: Udit Sharma and David Susnitzky, Evans Analytical Group.

B. PRD #2. Advanced Photovoltaic Analysis and Computational Modeling for Scale-Up

1. Problem Statement

Record photovoltaic cell efficiencies measured on small area cells (1 mm^2 to 1 cm^2) have historically not scaled well to production. In some cases, demonstration of record efficiency has not even led to a manufacturable, high-yield, large-area technology. Little is understood about the basic science of scaling a mm^2-device to $meter^2$ (m^2) or more.

2. Executive Summary

A well-established scientific framework addressing the challenging task of scaling from laboratory results to large area modules will benefit the photovoltaic industry by providing systematic understanding and design methodology to support rapid product introduction of photovoltaics into the U.S. energy supply. The industry need and scientific challenge are to achieve a basic understanding of issues critical for scale-up, such as defect structures and doping, especially in emerging materials such as multicomponent thin films such as cadmium telluride and CIGS, organic photovoltaics, and nanocrystalline photovoltaics. This is especially true for scaling to the large area and very high throughput needed for terawatt photovoltaic production. Basic research into the development of coupled analysis and computational methods addressing these critical issues is needed. Potential impact is a major advance in the competitiveness of emerging photovoltaic technologies, enabling broad application and allowing rapid transition of new technologies to large-scale economic production.

3. Industry Need

As the photovoltaic industry envisions scaling to the terawatt scale, it is clear that a number of key areas will need to be addressed. Even for crystalline silicon, not all critical basic science information is known nor are fully robust models available for the production process. The scientific foundation for scale-up of microcrystalline or thick film silicon on glass is not well understood. Thin film technologies such as CIGS and cadmium telluride are only poorly understood at the fundamental level, and emerging technologies and materials such as organic photovoltaics, copper zinc tin sulfide (CZTS), and quantum dot-based devices lack fundamental understanding altogether. This lack extends to the atomic and electronic defect structures, how doping affects the materials, and how defects and doping are related to process parameters, ultimate device performance, and stability. For rapidly expanding the production and insertion of existing and new systems, development of this understanding is critical.

This problem is of increasing importance as the diversity of photovoltaic products increases. Historically, silicon represented the vast majority of photovoltaics sold, but recent data indicate that the thin film market segment will be increasing rapidly. Significantly improving silicon production and facilitating the development of large-scale thin films and new technologies will clearly take a deeper understanding of the nature of the materials and interfaces coupled with analytical approaches for up-scaling to large areas. As this basic understanding develops, computational modeling of the materials, devices, and interfaces will allow for a much more rapid transition to large-scale manufacturing. This is especially critical for accelerating the deployment of new materials to avoid the traditional 30-year technology development path.

4. Scientific Challenge

The scientific challenge is to create a predictive loop between measurements with modern analytical tools and computational modeling that facilitates a more rapid development of photovoltaic materials and their transition to manufacturing.

CIGS cells are a perfect example. The best cells are made off-stoichiometry with a deficiency of copper, and with a gallium gradient throughout the cell. Sodium diffusion through the back molybdenum contact is critical, and the junction is made with a chemical bath-deposited cadmium sulfide layer. In fact, the basic science of nearly every one of these materials is not definitively known, yet CIGS cells are already in production. Organic photovoltaics are another example; as the drying temperature goes from room temperature to 180° Celsius (C) the complex morphology between an organic donor such as a polythiophene and a fullerene acceptor changes, and the efficiency can vary by more than 2%. Changing simple process variables changes the chemical nature of the polymer, the ordering mechanism, and the interface behavior.

Overall there is a need to begin to apply the suite of analytical tools at BES user facilities (see Chapter 11) to look at complex nanostructures structurally, optically, and chemically. These powerful measurement tools will provide the basis for developing a basic understanding which, when coupled to computational modeling, will enable rapid optimization of materials and devices, the development of in situ diagnostics and scalable processing.

5. Research Directions

- *Application of analytical tools to photovoltaic materials and interfaces,* in order to understand relationships of defects, doping, and processing, and their effects on ultimate performance. Electrical, elemental, and structural relationships can be deduced by coupling elemental analysis done with analytical tools such as secondary ion mass spectrometry (SIMS), local atom probes (e.g., see Fig. 3-6), and X-ray fluorescence to electrical measurements done with techniques such as capacitance-voltage spectroscopy, deep-level transient spectroscopy, and Hall probes [14]. Information determined from these electrical measurements such as diffusion length, majority and minority carrier concentration and lifetime, diffusivity and electric field distribution can then be related to dopant and defect levels in the bulk and at the interface. Additionally, there needs to be more development of large-area, rapid analytical tools.

- *Translation of analytical results to predictive models that address the cell to module gap.* Predictive models include quantum-chemical simulations for understanding atomistic effects in the materials as well as at interfaces and continuum models for prediction and understanding at the device to module level. In order for these models to be accurate, thorough parameterization is needed. This includes treatments of optical properties such as index of refraction and the extinction coefficient across the spectrum; electrical properties such as carrier diffusion lengths and lifetimes; mechanical properties such as thermal expansion and adhesion of different layers; thermal behavior of the electrical and mechanical properties between −20°C and 100°C; and environmental properties such as oxygen and water diffusion. The ultimate goal is to use these models to develop new materials, develop new diagnostic tools, and predict device performance and lifetime.

- *Development of a basic understanding of the materials, devices and processing to ensure scalability and replicability of production.* This understanding must be translated from the laboratory cell to a module and ultimately to a fully packaged system. For example, electrical and interfacial properties of the leads and busbars need to be understood at different lengths and thicknesses, since the diffusion of dopants is highly dependent on processing and edge effects change with scaling. Analytical tools such as secondary ion mass spectroscopy (SIMS) and scanning probes such as atomic force microscopy can be used to make measurements at different locations on a the substrate, cell or module. The results can then be correlated with electrical and structural properties studied at the nanoscale.

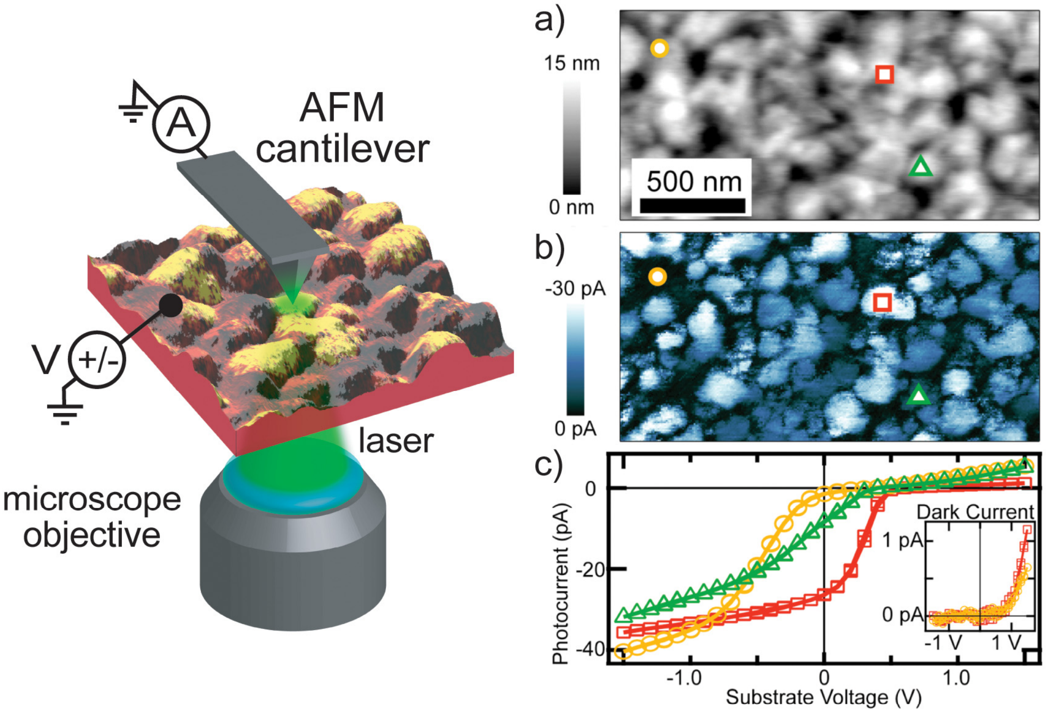

Figure 3-6 Scanning probe methods such as photoconductive atomic force microscopy (pcAFM) can be used to image the effects of nanoscale morphology on the performance of solar cells. A metal-coated AFM probe simultaneously recorded a) topography and b) photocurrent of a polymer/fullerene blend showing local variation in photocurrent collection efficiency associated with different domain structures. c) The local variations in short-circuit current are correlated with variations in the local current-voltage (J-V) curves that were acquired at the three locations. Source: C. Groves, O. G Reed, and D. S. Ginger 2010

6. Potential Impact

Advanced analysis and modeling would bring quantitative and predictive understanding to what is at present empirical optimization of photovoltaic systems. Basic understanding coupled to a robust computational framework would provide unprecedented tools for producing photovoltaics at high yield, on large areas at low cost. In particular, this would lead to improved performance, lifetime and production of existing technologies such as silicon; more rapid scaling of emerging thin film technologies such as cadmium telluride, CIGS, and copper-zinc-tin sulfide (CZTS); more rapid assessment and transitioning of emerging technologies such as organic photovoltaics to production.

C. PRD #3. Photovoltaic Lifetime and Degradation Science

1. Problem Statement

For photovoltaics to provide a significant contribution to the U.S. energy mix with a 2020 time horizon, the technology must be cost-effective with a rapid insertion rate and long lifetime. To achieve this we need fundamental advances in our understanding of photochemical, electrical and mechanical degradation under realistic solar insolation and thermal conditions. We also need to develop sufficient confidence in our basic understanding to support 25+ year lifetimes without 25+ years of testing.

2. Executive Summary

The industry needs advances in photovoltaic lifetime and degradation science in order to achieve higher reliability that will enable lower cost, faster technology insertion, and accelerated adoption of new technologies at a lower risk. For example, arresting thermal, electrical, and mechanical adhesion degradation processes, which reduce carrier lifetimes, degrade cell and module interconnections, and give rise to dielectric degradation and electrical shorts, will increase photovoltaic lifetimes. Research on photovoltaic lifetime and degradation will benefit from data mining of in-use performance of photovoltaic panels to establish the baseline experience and the common failure modes. In addition, devising accelerated tests with predictive performance metrics would enable evaluation of lifetime and degradation performance prior to installation.

3. Context and Background

The degradation rate of photovoltaic performance directly affects the levelized cost of electricity, which includes the capital and operating costs and the electricity production in each year of operation averaged over the lifetime of the system. The lifetime of photovoltaics placed in harsh exterior conditions under strong solar irradiation is dictated by the rate at which photovoltaics degrade by photo-thermal, thermo-electrical, and thermo-mechanical processes and mechanisms. Photochemical, electrical, and mechanical degradations produce a progressive decrease in power output and may result in abrupt failure. After an initial period, power degradation rates vary from

0.3% to 3% per year, highlighting the opportunity to dramatically decrease the levelized cost of photovoltaic electricity by increasing lifetimes. Reduced photovoltaic lifetime may be caused by shattered glass or back-sheet delamination (thermo-mechanical degradation e.g., see Fig. 3-7); cell hot spot formation (thermo-electrical degradation); or encapsulant discoloration (photochemical degradation). Some photovoltaic technologies, such as crystalline silicon, have “in the field” use histories, which provide long-term in-use experience that can be useful for identifying degradation mechanisms and failure modes.

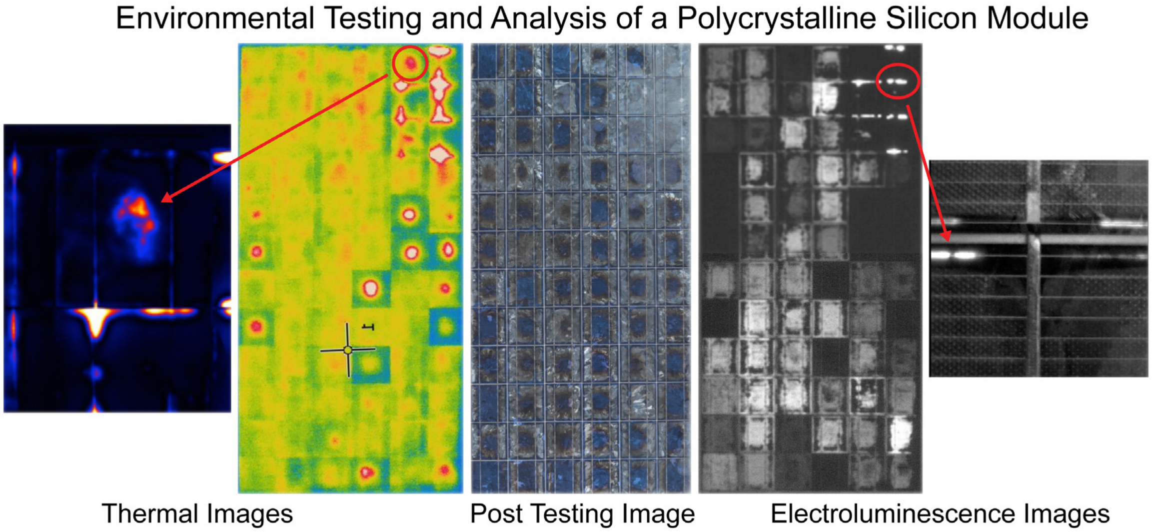

Figure 3-7 Failure analysis tests on a polycrystalline silicon module showing shunting in the middle of the cells and degradation of the Si-Ag electrode interface. Damp heat test was performed for 1,000 hours at 85°C and 85% relative humidity with –600 V system voltage applied to the active layer to accelerate hydrolytic and corrosive action of hot humid environments. Source: P. Hacke, National Renewable Energy Laboratory, http://www1.eere.energy.gov/solar/pdfs/pvrw2010_hacke.pdf.

4. Industry Need

Photovoltaic lifetime and degradation science must be developed to capture the photovoltaic opportunity. Many current efforts are focused on the initial performance of photovoltaic technologies to promote their first sale; however, the maximal benefit can only be attained from maximizing the performance of photovoltaics over their full lifetime.

Our ability to predict, control, and extend the lifetime of photovoltaic technologies with increased reliability is restricted by the challenge of forecasting the performance of complex materials systems over a lifetime that is much longer than typical technology development cycles. A fundamental and predictive understanding through photovoltaic science will allow the necessary control, which is essential to harness photovoltaics from initial performance forward.

5. Scientific Challenges

A photovoltaic module is a complex assembly of many different types of materials with many interfaces and structural components, enabling a failure of one component to disable the entire system (e.g., see Fig. 3-7). Examples include adhesion failure, delamination, and — highly relevant for many types of photovoltaics — the penetration of oxygen or moisture that accelerates photo-oxidation. Our scientific understanding is challenged by the very long lifetime required of photovoltaic technologies and the negative impact of even very slow thermo-mechanical degradation. Photochemical degradation of polymeric materials used in photovoltaic packaging and encapsulation affects both transparent optical materials in front of the active photovoltaic cell material and the non-optical materials, such as the backsheet behind the cells in a crystalline silicon module. A simple example is the behavior of non-active polymers used in photovoltaics for encapsulants. The materials must be solar-radiation-durable to resist photochemical darkening over the lifetime of the photovoltaic module. However, most of these polymer grades are developed in an empirical manner, as opposed to being designed to avoid the fundamental degradation processes. A scientific basis for future development of more complex materials, such as real encapsulants, adhesives, flexible packaging materials, or the new active organic photovoltaic materials, is also lacking.

Establishing the mechanism for thermo-electrical degradation of the active photovoltaic cell materials, conductors, and interconnects is also an important research challenge. For the highest photovoltaic cell efficiency, long carrier lifetimes are required, but in many novel compound semiconductors, both inorganic and organic, the science of carrier lifetime is in its infancy. We know that leakage currents degrade photovoltaic performance, that ion/charge migration can be associated with degradative processes and reliability, and that there can be dielectric degradation of insulating materials, especially under the high voltages that can be present in photovoltaic systems, but we cannot yet predict these degradation processes with certainty.

6. Research Directions

Photovoltaic cell and module efficiency has been the focus of most research. Efficiency investigations should be coupled with photovoltaic lifetime studies through examination of fundamental degradation mechanisms, pathways, and rates in materials, and at heterogeneous interfaces. We need to understand degradation mechanistically and identify methods, preferably intrinsic, to control or stop these degradative processes.

- *Investigation of the mechanisms for photodegradation of complex polymers used for active layers, encapsulants and front- and back-sheets.* Polyethylene-vinyl acetate is the most commonly used encapsulant material for photovoltaic modules, due to its low cost and good optical transmission. However, exposure to extended ultraviolet light and wide temperature ranges (below −15°C to 80°C or more) causes polyethylene-vinyl acetate to decompose. For concentrated photovoltaics, high solar flux (equivalent to 500 to 1000 suns) and high temperatures (greater than 70°C) can cause bubble formation, yellowing, and polymer decomposition in the silicone encapsulants. More studies are needed that correlate polymer degradation with outdoor conditions and field performance. Some of the possible tests include accelerated ultraviolet/humidity/thermal testing, rheological measurements, and thermal cycling. Additionally, the mechanisms associated with these degradation events in currently used polymers and new materials such as polymer-inorganic composites need to be investigated. Analytical techniques for such studies include modeling, chromatography, mass spectrometry, and nuclear magnetic resonance (NMR) spectroscopy.

- *Investigation of the photochemical, thermo-chemical, and thermo-mechanical stability of complex heterostructures at the nanoscale.* Nanoscale processes within photovoltaic cells and at interfaces are key to overall device stability. For wafers of crystalline silicon, understanding corrosion, cracking caused by mechanical and thermal strain, and developing the capability to make long-term predictions about these and other failure mechanisms are high priorities. Cell cracking can be studied by methods such as electroluminescence and infrared microscopy. Both thin-film silicon and cadmium telluride cells can suffer from electrochemical corrosion of the fluorine doped tin oxide transparent conducting oxide layer. By combining light soaking and voltage-biased damp heat tests, the corrosion mechanisms of this layer can be studied. For organic photovoltaic devices, photolytic instability, oxygen-induced and moisture-induced degradation, and thermal instability of donor and acceptor materials can cause drastic efficiency decreases. The origin of these instabilities — whether inherent in the active layers or due to unstable interfaces — requires much more understanding, with critical experiments ranging from reliability measurements on devices to spectroscopic and dynamic studies of the interfaces.

- *Investigation of the time dependent defect structure and ionic migration in multinary semiconductors and oxides.* Multinary semiconductors and oxide materials are widely used in the photovoltaic industry. Cadmium telluride and CIGS as well as other promising materials that use earth-abundant and non-toxic elements such as copper zinc tin sulfide, iron sulfide, copper sulfide and copper oxide are employed as the light absorbing layer in thin-film photovoltaics. Multinary oxides such as zinc oxide, indium tin oxide, and fluorine-doped tin oxide are used as window layers or transparent electrodes for many photovoltaic architectures. The high-efficiency multijunction cells (>40%) used in concentrating photovoltaics are composed of multiple layers of light-absorbing materials such as gallium indium phosphide, gallium arsenide, and indium gallium arsenide. In these existing and emerging materials, basic understanding of doping and defect structures within the bulk materials and across interfaces is needed. Parasitic trap states in the bulk, at interfaces, and at the surface are caused by irregularities such as point defects, dislocations, and impurities, and can significantly lower the device open-circuit voltage. Defect and dopant migration can also occur across interfaces. Investigations could include time-resolved spectroscopy studies, temperature-dependent experiments, modeling, and advanced characterization such as neutron powder diffraction, electron microscopy, and X-ray scattering and spectroscopy done at BES-funded user facilities.

- *Investigation of electrical shorts and dielectric degradation in packaged photovoltaic systems as a function of insolation, moisture, temperature and photo-bleaching.* Electrical shorts due to material degradation, pin holes, or structural defects can significantly limit the lifetime of a photovoltaic module, and a better understanding of degradation mechanisms is needed. For example, scanning probe microscopy techniques, such as conductive atomic force microscopy, Kelvin probe force microscopy, and scanning transmission electron microscopy can correlate electrical function with structures at the nanoscale. In situ experiments are possible with these techniques, for example, real-time heating and deformation experiments can be done using in situ transmission electron microscopy.

- *Development of an understanding of the mechanisms of interfacial degradation in photovoltaic devices and systems under real environmental conditions.* Many of the most critical processes in solar cells occur at interfaces such as p-n junctions, contacts, and tunnel junctions. The performance and lifetime of the cells are highly dependent on the stability of these junctions. Examples of destabilizing processes include interlayer adhesion and delamination in cadmium telluride, copper indium sulfide, and CIGS cell layers; instability of the metal/organic interface and transparent conducting interfaces in organic photovoltaics; and lattice strain of heterojunctions. Of special interest are lattice mismatched layers in III-V multijunction devices and between the active and window layers in thin-film photovoltaics. At the module level, delamination of busbars, failure of antireflective coatings on glass and the optics for concentrating photovoltaics, and packaging are issues that need to be understood.
- *Development of accelerated irradiation, temperature, voltage and humidity tests, with rate constants and fundamental mechanism-based models for realistic photovoltaic systems.* To understand the complexities of fundamental degradation mechanisms, tools need to be developed that can help probe these processes, especially at the cell-to-module level. For example, application of high voltages during damp heat exposure might uncover corrosion issues for modules in high-voltage systems. An infrared camera could be used in combination with damp heat exposure to understand busbar failure due to mechanical and electrical breakdown.

7. Potential Impact

The fundamental science of photochemical, electrical, and mechanical degradation of photovoltaic technologies under realistic solar insolation and thermal conditions would provide the foundation needed to assure the long lifetimes for multiple photovoltaic technologies. This would benefit the development and insertion of current and new photovoltaic technologies in three ways:

- *Photovoltaic efficiency and reliability.* Improvements that limit or eliminate degradative processes can contribute to energy output and reliability and reduce the inherent risk in photovoltaics, improving their adoption and insertion rates.
- *Photovoltaic lifetime.* A sound scientific basis for understanding and controlling photovoltaic degradation processes would allow the optimization of materials and designs for long lifetimes, lowering the cost of electricity averaged over the lifetime of the system.

- *New photovoltaic technologies.* Degradation science could be leveraged and applied to novel photovoltaic technologies, which may have good initial device performance results, but as yet, lack the history needed for predictable lifetime and reliability.

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Chapter 4: Panel 2 — Advanced Nuclear Energy
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Panel Members:
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- William Barletta, MIT
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- Michael Burke, Westinghouse
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I. EXECUTIVE SUMMARY

There is a growing consensus that large carbon dioxide (CO_2) reductions and energy security with stable supply and prices for electricity cannot be achieved without a major contribution from nuclear energy. It remains the single largest contributor of non-CO_2-emitting electricity, ultimately providing more than 70% of the non-emitting energy-generation capacity in the U.S. The contribution of electricity from nuclear power will need to increase in the coming decades in order for the U.S. to meet CO_2 reduction targets while maintaining reliable, low-cost energy. Although nuclear power is generally considered one of the most scientifically intensive of all forms of energy generation, the basis for designing, building, and operating our current plants is largely empirical. Therefore, this area could benefit significantly from increased scientific sophistication. More specifically, the Workshop panel suggests three priority areas where basic science can significantly improve the reliability and economics of current and next generation nuclear plants: an improved understanding of materials degradation mechanisms for components in the primary coolant system; a scientifically based ability to translate results from accelerated testing environments for 60 years and beyond in commercial reactors; and the scientific basis to support the ultimate solution for used fuel and high level waste.

II. PANEL REPORT

Role of Nuclear Energy

Nuclear power currently contributes about 20% of electricity generation in the U.S. Because of their low operating costs, including low fuel costs, nuclear plants are used almost exclusively in the U.S. to provide baseload generation. Once the capital costs of the plants are paid off, nuclear plants provide some of the lowest cost electricity in the energy generation mix. More recently, the attention on nuclear energy has shifted to its role as a non-CO_2-emitting source of clean energy, particularly when large-scale baseload generation is required, and also as a means ("load following") to offset generation variability in regions where there is substantial penetration of renewables like solar and wind.

Nuclear power is increasingly seen as a necessary part of our energy generation portfolio in a carbon-constrained world. A number of studies have concluded that the U.S. will not be able to reach the targets for CO_2 reduction without a full portfolio of non-emitting forms of energy generation, including nuclear. The example shown below (Fig. 4-1) is the PRISM analysis by the Electric Power Research Institute (EPRI) [1]. It shows that with aggressive but plausible increases in all of the technologies, a 41% reduction in CO_2 emissions by 2030 is possible. For reference, the yellow band in the plot represents an additional 64 GWe of nuclear-generating capacity, which requires roughly 50 new plants. It also assumes no retirements from the current fleet, the importance of which cannot be overstated. Plants in the U.S. originally received licenses to operate for 40 years. A number of plants have already received licenses to operate for 60 years, while others are still pursuing their license extension as they approach the end of the originally licensed period. To keep the fleet fully operating to 2030 and beyond, the industry will need to license currently operating plants to lifetimes of 80 years or more.

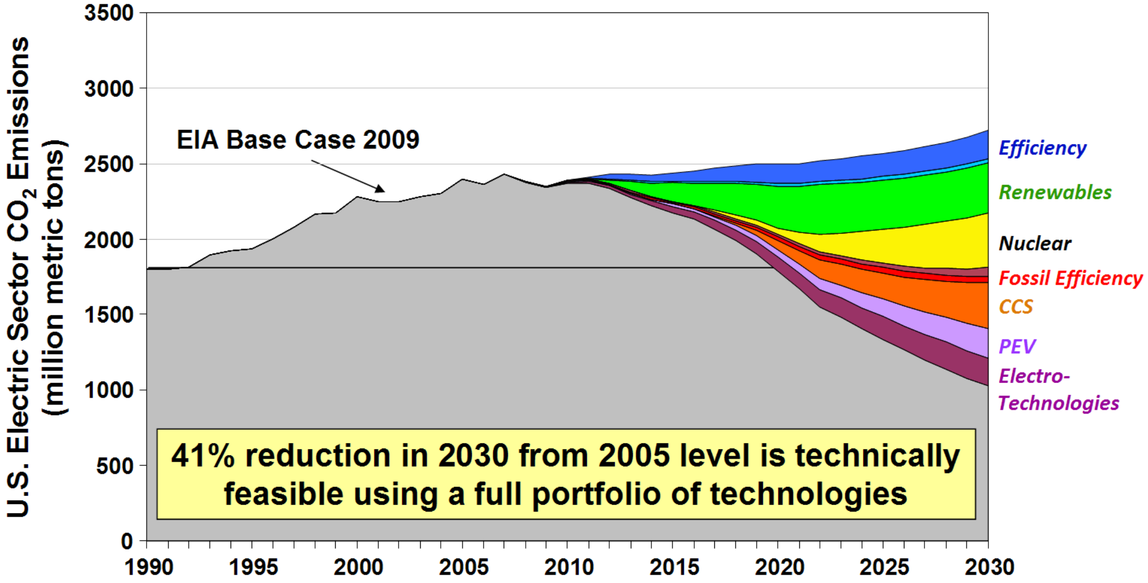

Figure 4-1 PRISM analysis showing potential reduction in CO_2 possible with aggressive implementation of a full portfolio of generation options. Source: EPRI

Status of Nuclear Power and Technology Gaps

Since the first commercial nuclear plant in the U.S. began operation at Shippingport, Pennsylvania in 1958, the industry has continued to improve plant design and operation through a long series of technology improvements. Even over the past two decades, the industry has seen substantial improvements. The energy extracted from the fuel ("burnup") has more than doubled; the plant capacity factor (percentage of power generated relative to 100% continuous operation, see Fig. 4-2) has increased by 20 to 30%; and the licensed power ratings of existing plants have increased by the equivalent of almost 6 GWe in capacity [2]. At the same time, the safety record of these plants has never been better.

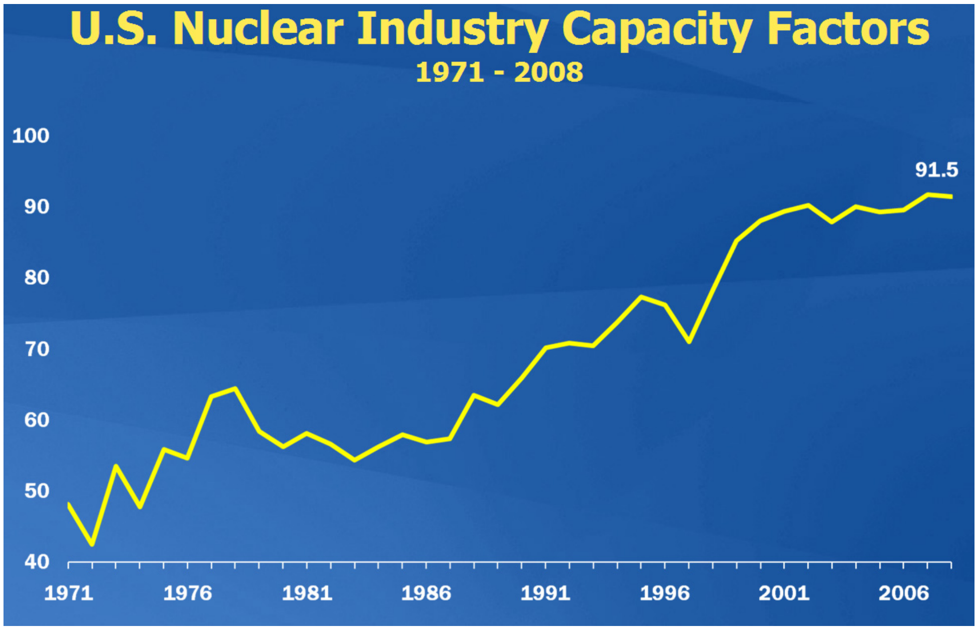

Figure 4-2 Capacity factor (shown as percentage of maximum generation) in the U.S. nuclear industry. Source: Nuclear Energy Institute.

This is not to say that all of the issues related to nuclear power have been solved. A number of critically important areas require active research and additional understanding of the basic science.

For example, many point to the absence of an accepted solution for the waste generated. Although the volume of waste is actually quite small considering the scale of nuclear power generation, waste management is an important area for the industry, one that could benefit more from advances in science than from incremental improvements in engineering. A better understanding of actinide chemistry would be a major scientific contribution, enabling the design of better waste disposal or recycling solutions. Actinide chemistry is the focus of one of the priority research directions suggested in this report.

Another area of industry focus is assuring and extending the lifetime of the existing fleet of light water reactors (LWRs). Scientific understanding of materials degradation over long time periods is critical to achieving this objective. In particular, extending the lifetime involves managing the integrity of the key barriers to radioactive release, namely, the fuel cladding, the pressure vessel and primary system components, and the secondary containment. A simplified schematic of a pressurized water reactor (PWR) is shown in Fig. 4-3. The other common commercial reactor design, the boiling water reactor (BWR), would appear similar at this level of detail except that steam is generated directly from the reactor vessel.

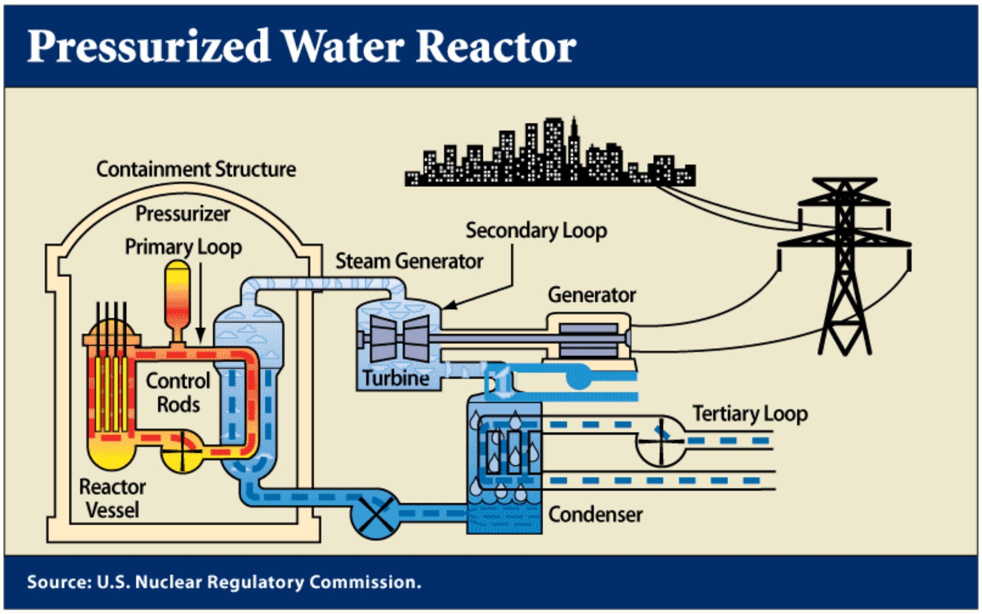

Figure 4-3 Schematic of a pressurized water reactor. Source: U.S. Nuclear Regulatory Commission.

The first barrier to radioactive release, the fuel cladding that separates the ceramic fuel and fission products from the coolant, is an important area of focus, and the industry has made substantial improvements in the performance and reliability of nuclear fuel over the past several decades. For example, most plants today are able to operate complete cycles (18-24 months) at full power without a single failure in the roughly 50,000 fuel rods. In a continuous drive for excellence, the industry plans to persist in their efforts until every plant routinely operates without a single failure. While most of the immediate challenges are operations- and engineering-related, there are important science challenges, particularly as related to enabling revolutionary fuel designs such as high-temperature ceramic claddings; high-power, high-conductivity fuels; or coolant additives to increase heat transfer.

The second barrier to radioactive release, the pressure vessel (also referred to as the "reactor vessel" as shown in the figure) and other pressure boundary components, has seen substantial progress in the industry's ability to identify and mitigate issues that pose a challenge to pressure boundary integrity. Like many aspects of the nuclear industry, the basis of our technical understanding is almost entirely empirical. A more fundamental scientific understanding, including the evolution of materials properties under irradiation and degradation mechanisms that affect structural components, is urgently needed to enhance our overall ability to manage the current fleet and to design the next generation of commercial reactors.

The third barrier to radioactive release, the containment structure, is receiving an increasing amount of attention. Our need for scientific understanding in this area, concrete degradation in particular, will only grow in importance as reactors approach the end of their licensed life, and the industry seeks to provide a technical basis for extending plant lifetimes from 40 or 60 years to 80 years and beyond.

Power uprates (literally increasing the amount of power achievable from a currently operating plant) almost always represent the most economic form of additional nuclear generation. The power level of a plant is typically increased through an improved analytical understanding of plant conditions and equipment limits, and from upgrades to the plant equipment (steam generators, turbines, etc.) and fuel. It is important to acknowledge that one of the reasons power uprates are so attractive is that the capital cost for new nuclear plants is high. In fact, capital cost is possibly the biggest challenge for nuclear power, although this workshop panel did not identify research directions aimed directly at reducing capital costs (which were perceived to be more engineering and procurement issues than science issues, at least for the current LWR technology).

The industry is now on the verge of building a new generation of LWRs. These reactors include additional features to make the plants even safer and more efficient. It is important to note that the basic technology needs of the current fleet and next-generation nuclear plants are very similar. Therefore, any advances in technology will positively impact the U.S. for the next century or more.

To summarize, several areas related to nuclear power could benefit from a stronger fundamental understanding of materials, the changes they undergo in the nuclear reactor, and the degradation mechanisms affecting safe and economic operation. The topics include degradation of many components of the reactor core and primary system, as well as aspects related to the back end of the fuel cycle.

Potential Research Directions

The panel considered a number of important research directions to which Basic Energy Sciences (BES) could make significant contributions, including design of advanced fuels capable of higher power and higher burnup; creation of sensors capable of directly monitoring in-reactor performance; and development of advanced non-destructive evaluation techniques that could detect the onset of materials degradation. Three priority research directions address important challenges for nuclear energy and play particularly to BES strengths. The first priority is to develop a fundamental understanding of materials degradation mechanisms. While this area has been the focus of intense study over the past several decades, a higher level of sophistication is needed to address this highly complex problem. The second priority is to develop detailed scaling laws between commercial reactor environments and those of test facilities. Such an understanding would facilitate accelerated testing to predict materials performance across plant lifetimes of 80 years or more; it would also directly benefit studies on materials degradation mechanisms. The third priority is to increase our fundamental understanding of the back end of the fuel cycle. A number of fundamental properties of the fuel will be important regardless of the particular approach ultimately chosen for storage, reprocessing, or final disposition.

The BES community and national laboratories in the Office of Nuclear Energy programs compiled a report [3] on research directions that bear directly on and are well aligned with the priority research directions identified in the present report.

III. PRIORITY RESEARCH DIRECTIONS

A. PRD #1: Materials Degradation Mechanisms

1. Problem Statement

All currently known structural materials degrade under nuclear plant operating conditions to the point that they need to be replaced, repaired, or extensively monitored over the life of the plant. A fundamental understanding of the degradation processes, particularly those associated with fracture and stress corrosion cracking, would support the development of advanced approaches to

1. Accurately predict component lifetimes and manage the materials issues in the current fleet,
2. Inform development of a licensing basis grounded by fundamental understanding, and
3. Develop new materials for plant repair and life extension as well as for insertion in next generation plants.

2. Executive Summary

Materials degradation is the key issue for nuclear power relative to maintenance and operation of the current fleet, extending plant licenses to 80 years or more, and identifying important improvements for the next generation of plants. Utilities will make multi-billion dollar investments and need absolute confidence in the supporting science. Understanding the mechanisms of degradation is a daunting scientific challenge. However, it is clear that developments in experimental and modeling capabilities will radically change the way the industry licenses and operates the plants. In particular, advanced modeling capabilities coupled with carefully controlled, high-fidelity experiments should lead to a major advance in our understanding of the most important degradation mechanisms.

3. Background

Materials degradation and management is the key issue in assessing and extending plant life. U.S. plants were originally licensed for 40 years, based on the data available in the 1960s. At that time, pressure vessel integrity was targeted as the key materials degradation issue and licensing relied upon vessel surveillance coupons retrieved at various times to assess changes in materials properties over the plant's operational lifetime. The results from these surveillance coupons, combined with investigations on other irradiated components, have formed the basis of licensing plant operation to 40 years and, in some cases, to 60 years. However, no such provisions were made to follow the degradation of the less sensitive but more highly exposed materials that make up the core internal structure. Fundamental studies of irradiation damage, often in model alloys, have supplemented our understanding of degradation phenomena, but have not greatly influenced the 60-year licensing approach. With the industry now looking to license plants for 80 years and beyond, this approach needs to change. Given the more severe conditions that reactor materials are expected to endure, the understanding must be broadened to encompass the materials employed in the structural internals, as well as those employed in the pressure vessels.

4. Industry Need

The industry's greatest need is addressing plant lifetimes and supporting plant life extension. Improved precision and reduced uncertainty in life prediction would follow from a better understanding of materials degradation mechanisms and from improved, mechanistically based models of material evolution. This advanced understanding would be combined with a more extensive database for better predictions.

More specifically, the industry needs to know which features of the microstructure and microchemistry influence the mechanical response of commercially operating components and how materials can be manipulated to mitigate deleterious effects. Industry also needs to know when these features are present, how they can be expected to evolve, and how they might synergistically interact (Fig. 4-4). Models for such systems will necessarily be complex; so the industry will also need to know how or whether such models can be simplified for application in engineering and licensing tools and what uncertainties arise from the simplifications. The quantification of uncertainties is central to using fundamental approaches to materials performance.

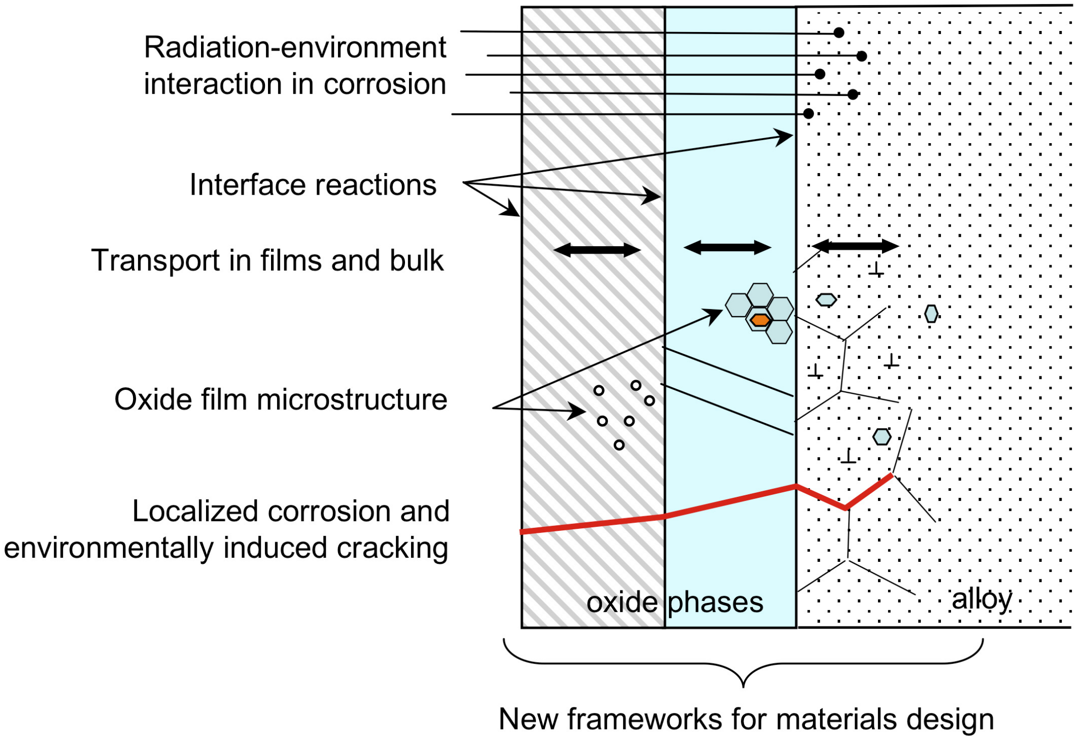

Figure 4-4 Schematic of interactions between materials and environment in structural alloys. Source: Gary S. Was, University of Michigan.

5. Scientific Challenges

Although our understanding of microstructural changes and material degradation mechanisms in LWR environments has improved substantially over the past several decades, the scientific challenge ahead is still daunting as we strive for prediction capabilities with the highest possible resolution. The fundamental challenge is to understand detailed materials and chemistry effects on degradation. Current databases of irradiated materials properties are not adequate to support predictive models. Specific scientific challenges include:

- Understanding microstructural and microchemical evolution under prototypic LWR neutron spectra,
- Developing approaches to properly combine models for assessment of simultaneous degradation modes,
- Assessing uncertainties from a fundamental, science-based viewpoint,
- Assessing actual materials with inherent (and often unknown) variability, and
- Scaling from one set of irradiation conditions to another (see next PRD).

6. Research Directions

The overarching directions for this research are as follows:

- Establish quantitative correlations for effects of irradiations on materials properties and
- Develop more comprehensive modeling capabilities, with increased precision and fidelity, to follow irradiation-induced materials degradation over the full life of the in-service use of the material.

Because commercial alloys are multi-component materials that undergo complex interactions with the reactor environment (both the energy fields and the coolant), early stages of this effort should start with a carefully chosen set of commercial alloys. The research team would work with industry on characterization and modeling techniques to identify the most important features for further study. Simpler model alloys could then be produced, irradiated, and examined to address the more fundamental questions, in close coordination with the modeling effort. Modeling could include techniques such as:

- Molecular dynamics and other ab initio approaches to understand defect formation, migration, and interaction, coupled with classic thermodynamic and kinetic models as needed,
- Models for fracture, corrosion, and stress corrosion cracking,

- Multi-scale approaches in both length and time scales, and
- Monte Carlo approaches to define uncertainties.

7. Potential Impact

This priority research direction could transform the operation and design of LWRs, affecting the decisions the nation makes on how long the current fleet can be safely operated, how many new plants should be built, and for how long they can be licensed. More specifically, the research outlined here would be expected to:

- Quantify plant lifetime predictions, a prerequisite for reactor life extensions,
- Quantify margins and evaluate the case for power upgrades,
- Quantify the impact of coolant chemistry changes on service durability and possibly suggest novel approaches to mitigating materials degradation,
- Guide development of key inspection practices and ensure the industry is focused on the highest priority areas, and
- Identify and design new materials options for future reactors.

B. PRD #2: Scaling of Advanced Irradiation Effects

1. Problem Statement

The expense and time necessary to bring new and improved nuclear technologies to market impede the progression of nuclear energy to higher efficiency and lower cost. Advanced experimental techniques can be applied to this end in innovative ways, if the conditions and scales of the techniques can be appropriately extended to the in-service conditions they seek to address. Developing these techniques and establishing their scientific basis require contributions best made by the BES community.

2. Executive Summary

Basic and quite challenging research is needed to develop and technically justify innovative approaches for understanding irradiation damage in materials and key materials degradation mechanisms. This research would change the manner in which reactor fuels, structural materials, and coolant operating regimes are studied, developed, and brought to market. A key principle in this effort is the scaling, or extension, of laboratory experiments and data to actual in-service conditions. Advancement in scientifically rigorous understanding of the scaling rules for irradiation phenomena is required to properly develop the accelerated testing that is needed to support the development of new materials for long-life reactor service. If cost and duration of technology development can be reduced through application of modern modeling and accurately scaled and interpreted with experimental data, then barriers to bringing improved technology to market will be reduced and technology solutions that greatly enable advanced systems, such as fast reactors and fusion energy systems, may emerge.

3. Background

Efforts to develop and license new technology for nuclear energy applications require long durations and substantial cost. The empirical nature of previous R&D programs, though successful in developing technology that is commercially deployed today, are increasingly challenged by the nature of today's performance objectives (typically trying to achieve higher performance under more severe conditions), by the disruption in continuity of federal and industry nuclear energy R&D during the 1990s, and by the escalating cost of maintaining specialized facilities necessary to work with nuclear materials. The technologies normally addressed in this manner (e.g., fuel and cladding, structural materials, coolant chemistry) are also those that most affect the safety and performance of nuclear power plants, so improvements in nuclear energy must address those technologies. Researchers and technologists have long sought to make such R&D programs more efficient and effective through application of predictive modeling capabilities that inform and focus experiments. However, the complex nature of the phenomena and the limited mechanistic fidelity of the models applied to those phenomena discouraged real progress through that approach. Recent developments with advanced modeling techniques and high-performance computing offer hope for a paradigm change, enabling breakthroughs through better mechanistic understanding of phenomena, as well as simply shortening the time to identify promising developments.

Licensing times would also benefit from a demonstrated scientific understanding of the performance and degradation phenomena associated with new technology; recent experience with regulatory agencies indicates that licensing times are strongly affected by the time required for performance demonstration of new technologies under actual in-service conditions to resolve uncertainties and provide assurance that performance is as expected.

4. Industry Need

Industry needs modeling and experimentation techniques that enable mechanistic-based approaches to technology development. More specifically, precise models are needed to support technology decisions based on macroscopic properties associated with:

- Time dependence of irradiation damage and accommodation of fission products in fuel and structural materials (i.e., evolution of microstructural and microchemical characteristics) and
- Time-dependent chemistry of multiphase fluids, including radiolysis.

Given that the techniques and approaches called for necessarily make use of experiments that are not conducted in commercial power plants, industry further needs a sound and defensible case for the relevance of these techniques to actual service conditions. This need will require predictability across diverse irradiation spectra (thermal to fast to accelerator based) and means to scale test data to in-reactor performance. Past experience has shown that acceleration of testing, e.g., by higher flux conditions, tends to increase damage accumulation effects. Experience to date indicates that the present state of the art provides undesirable uncertainties and excessive conservatisms. Accelerated testing protocols that are founded on reliable extension-of-scale scientific principles are needed to support the analyses of existing and future materials.

5. Scientific Challenges

The models needed to sufficiently characterize the phenomena are necessarily complex, addressing effects of temperature and radiation (as well as other specific deployment conditions such as stress or changing coolant species) in multi-component systems (such as engineering materials and dynamic coolant chemistries) over wide ranging time scales (perhaps pico seconds for fundamental irradiation damage mechanisms, but extending to decades when predicting component performance over the plant's lifetime). It is essential that this effort lead quickly to approaches that can be deployed with engineering materials. Complex interactions between materials and environment are difficult to simulate in experiments outside of the actual application, so the mechanisms operative in the actual environment must be identified and isolated for reproduction and measurement. Extension of short-time high-rate experimental data to longer-term low-rate phenomena, such as materials degradation phenomena operative over 80 years, will be difficult. Finally, to address industry needs, predictions of models developed in this manner must be validated against actual or prototypic performance data, with uncertainties quantified in a manner that can be incorporated into larger predictive codes.

6. Research Directions

The *Basic Research Needs for Advanced Nuclear Energy Systems* report [3] articulates many relevant approaches suitable for BES research programs. It is important to reiterate that industry objectives are not met if the developed techniques are not extended beyond single component or binary systems to engineering materials and systems. However, the following general directions are suggested:

1. *Experimentally characterize, irradiate, and model a prioritized set of controlled materials in multiple environments*. Well-defined irradiation experiments are envisioned, using characterized ion beams (including multiple ion beams) and available neutron irradiation tools. Environmental effects, such as high-temperature water (single phase or two phases) with important chemical species and radiolysis effects or hydrogen-rich atmospheres typical of fusion applications, should be incorporated systematically. The effects of radiation and environment on the microstructure and properties of test materials can then be characterized and compared with those of materials taken from actual or prototypic environments, with key experimental parameters identified for further study.

2. *In parallel, develop and validate multi-time and spatial-scale computational models*. Modern modeling approaches (e.g., ab initio molecular dynamics or other meso-scale

approaches) will be applied to the mechanisms isolated for study in the experiments described above. As those models are developed, certain physical parameters will likely emerge as data needs, which can then inform and focus the experimentation.

3. *Provide direct link between test facilities and irradiation damage*. Establishment of the test methods, which provide a basis for application of experimental data to justify industrial technology development and to support subsequent licensing, will require a scientific basis that links predictive models to in-service performance of reactor components or systems. The uncertainties inherent in the measurement and prediction methods themselves must be identified.

7. Potential Impact

The envisioned work will provide validated techniques for applying available test facilities to evaluate the behavior of reactor fuels, materials, and coolant outside of actual in-service environments. Knowledge and understanding obtained using these approaches can then be used for accurate plant lifetime prediction and life extension. Such techniques will also accelerate innovation and down-selection of design and material options, thereby reducing development times to bring new materials to market.

Although the benefits of these Priority Research Directions are couched in terms relevant to today's nuclear energy industry, the Panel advises that the work envisioned addresses not only thermal LWRs but also high-temperature gas-cooled reactors, fast reactors, and fusion energy systems. The modeling and experimental approaches, and likely the specific models of behavior that are enabled, will be applicable to materials and design efforts for those more advanced systems.

C. PRD #3: Back End of Fuel Cycle

1. Problem Statement

The nuclear industry requires that technical options for the back end of the fuel cycle – dealing with spent fuel – be refined and not prematurely eliminated, while technology and policy decisions are made and implemented. This situation, in turn, necessitates that stewardship of this radioactive material be maintained for an indeterminate length of time while technology development is focused on shaping the decisions for a permanent solution. Progress on pivotal technological developments is restricted by insufficient fundamental understanding of the basic physics and chemistry of the actinide-bearing systems that comprise postulated separation intermediaries and fuel and waste forms in a recycling fuel cycle. More complete information is urgently needed for nuclear cross sections and for depletion and integral nuclear interaction effects to facilitate the increasing time of "temporary" storage on the reactor plant site and for the ultimate transportation of the used nuclear fuel.

2. Executive Summary

Advancing the use of nuclear energy will require that the back end of the fuel cycle be intelligently handled, and that both the fissile resources and waste streams be properly managed. These are preconditions to wider use of nuclear energy while maintaining proper security and safeguards worldwide. To quote John Rowe, President & CEO of Exelon, "We have to be able to look the public in the eye and say 'If we build a plant, here's where the waste will go'." The current situation is that plants will be storing used fuel at the reactor sites until final disposition is resolved.

To these ends active theoretical and experimental programs are necessary to research (i) closure of the fuel cycle, from recovery and waste processing to manufacture and operation of fuel containing at least a portion of the actinides created during fuel irradiation, and (ii) the problematic sequestration of radiotoxic fission products and interim disposition options for current forms of fuel being stored at reactor sites. The actinides and the remaining fissile and fertile content of used nuclear fuel represent a significant potential power-producing resource for the global energy market. Should a closed, sustainable fuel cycle not be pursued in the U.S., then the used fuel must ultimately be handled in such a manner as to immobilize its various constituents, at least in accordance with their characteristic radiotoxic lifetimes. BES's science leadership is required for progress in separation technologies (both electrochemical and aqueous), recycling (mainly fast neutron reactors), and actinide/fission product immobilization, and is a cornerstone for building this U.S. capability.

Fuel cycle research motivated in the 2006 report *Basic Research Needs for Advanced Nuclear Energy Systems* [3] will help meet the most urgent needs if it can be focused to address engineering systems of interest. Specifically, the chemistry and physics of actinide electronic systems are not well understood. Current computational electronic structure approaches are inadequate to describe the electronic behavior of actinide materials. The multiplicity of chemical forms and oxidation states for these elements complicates their behavior in fuels, solutions, and waste forms. Similarly, immobilization of many of the fission products in used fuel, when considering the difficulties represented by volatility, radiation damage, heat loadings, process stability, and durability requirements, challenges current understanding. Meanwhile, interim solutions for the storage and transportation of used fuel must be informed by sufficient scientific knowledge to not preclude technological choices further in the future.

3. Background

Developing and licensing new technology for nuclear energy application is a lengthy and costly process. The previous largely empirical R&D programs have been successful in developing the technology deployed today, but new challenges arise from today's sustainability objectives, from the disruption in continuity of federal and industry nuclear energy R&D during the 1990s, and from the escalating cost of maintaining specialized facilities necessary to work with nuclear materials. The isotope content of used fuel shows that while much of the U-235 is consumed during operation, some portion of the original fissile material remains, and additional fissile material is created (see Fig. 4-5). Long-term sustainability for the nuclear fuel cycle is envisioned through the "closing" of the fuel cycle by recycling used fuel material back into a nuclear reactor in order to extract additional energy. Closing the fuel cycle necessitates development of actinide-based fuels for advanced nuclear energy systems, which, in turn, requires new chemical separation strategies and predictive understanding of fuel and waste-form fabrication and performance. Maintenance of an open fuel cycle requires the stewardship of used fuel at reactor sites with a plan for final disposition in a geological repository.

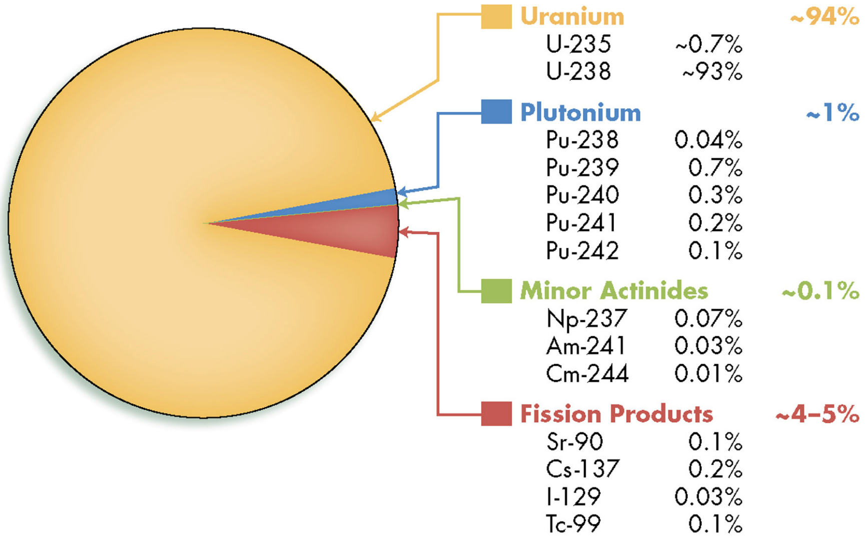

Figure 4-5 Typical fuel rod composition after discharge from reactor. Source: EPRI [4].

4. Industry Need

In order that informed technology and policy decisions are made and implemented, it is necessary to put in place those fundamental pieces of science that provide an understanding of the complex, multi-component system of actinide- and fission-product-bearing materials associated with all back-end options in the fuel cycle. Regardless of whether the fuel cycle is closed and the manner in which it is closed, requiring separations and recycling technology, or whether it is open, requiring prediction of the stability of the fuel in its current form, understanding of the basic physical phenomena of matter is needed in the areas of

- Chemical processes of separation,
- Chemistry and physics properties of actinide-bearing fuel forms (for recycling and long-term storage),
- Chemistry of final waste forms, and
- On-site storage and transportation implications.

5. Scientific Challenges

Insufficient knowledge of chemical bonding of actinide and fission product complexes limits prediction relevant to recycling (separations, dissolution, and stabilization of waste forms) and to media proposed for advanced processing systems. A scientific challenge is to develop a robust theoretical foundation for treatment of actinides and actinide-containing systems. Advances in exchange and correlation functionals in density functional theory (DFT), as well as in the treatment of relativistic effects and in software implementation on advanced computer architectures, are needed to adequately treat the behavior of 5f electrons in the actinides. Substantial progress has been made over the past few years toward a comprehensive theory. Recently, exact exchange and hybrid DFT approaches developed for molecules have been implemented for solids, and the limited experience obtained thus far suggests these approaches are promising. Small-scale physics experiments to elucidate the electronic structure and the fundamental properties of actinides will be required to guide and validate the theories.

Closing of the fuel cycle, while considered to be key to long-term sustainability of nuclear fission as a global energy source, will also involve separation of fission products from the used fuel, many of which are inherently difficult to immobilize and have a relatively high level of decay radiation, and so their sequestration is problematic for the hundreds or thousands of years required to reduce radiotoxicity to acceptable levels. The range of fission products covers halogens, ^{14}C, ^{99}Tc, ^{3}H, ^{137}Cs, ^{90}Sr, ^{85}Kr, and others, and may include actinides as well. The scientific challenge is to develop physical and chemical forms of fission products that

- Are radiation resistant with low solubility and
- Have low volatility and high temperature stability.

Both open and closed fuel cycles require addressing the scientific challenge of developing and validating an enhanced nuclear parameter description, especially in the validation of cross sections, for the coupled sets of actinides and fission products within fuel forms, as well as separations and waste streams. This task requires the reinvigoration of capabilities to perform individual and integral nuclear cross-section measurements, as well as critical facilities and appropriately equipped hot cells for accurate isotopic assay.

6. Research Directions

The reader is directed again to the 2006 DOE report on *Basic Research Needs for Advanced Nuclear Energy Systems* [3], which articulates suitable approaches for BES research programs. In particular, the following research directions are envisioned to achieve a better fundamental understanding of the properties (thermodynamics, kinetics, and mechanisms of separation processes) of complex, advanced actinide materials, especially at high temperature:

1. Developing electronic structure methods based on molecular orbital theory and density functional theory to address the f-electron challenge, including density functional theory and relativistic core potentials for structure and energetics of complexes with actinides in low oxidation states and with more than one 5f electron. [5,6] These approaches must improve the accuracy of property predictions for f-element-containing molecules and

solids (energetic, physical, magnetic, and spectroscopic) and must be capable of addressing the defect properties of multi-component actinide fuel/fission product systems to provide predictive capabilities for developing processing systems for separations design, accounting for unconventional phase behavior and stoichiometry, and going beyond the current qualitative descriptions (Fig. 4-6).

2. Developing electronic structure methods, for example, for first- and second-row compounds, providing essentially exact answers, even if only for model systems.

3. Developing nonconventional experimental techniques to measure the thermal dependence of the properties of complex actinide materials, especially at extreme temperatures. Such techniques will allow for the study of high-temperature phase equilibria and associated fundamental chemical and physical properties, which are not currently possible to determine by conventional techniques. Additional experimental measurements are needed to obtain high-accuracy thermodynamic, kinetic, and spectroscopic data for benchmark purposes, especially for radioactive elements.

4. Developing integral cross-section demonstration techniques, which are not necessarily possible in current critical facilities for radioactive, multi-isotope systems, to provide benchmarks for verification of criticality methods. This task includes benchmarking for depletion methodologies for determination of uncertainties to use in safety analyses of back-end fuel processing, storage, and transportation.

7. Potential Impact

This priority research direction addresses scientific obstacles to a final solution for used fuel, either through an open fuel cycle with permanent waste storage or a closed fuel cycle with recycling. It could set the stage for acceptance of current and near future LWR technology by removing a key obstacle to completion of its nuclear-fuel life cycle. Another possible impact is to more quickly and pervasively launch a "nuclear renaissance" in this country, as well as recover the national capability to lead an industry the U.S. originally created. Obviously, all the proposed research supports the regulatory pathway, an integral part of any nuclear energy development program. More specifically, the priority research would be expected to

- Provide key understanding to gain orders of magnitude improvement in sustainability of the nuclear fuel cycle by increasing fissile resource utilization,

- Gain public acceptance for nuclear fuel cycle solutions,

- Reduce the uncertainty for current storage and transportation, and

- Reduce the volume and risk of ultimate waste and effluent streams.

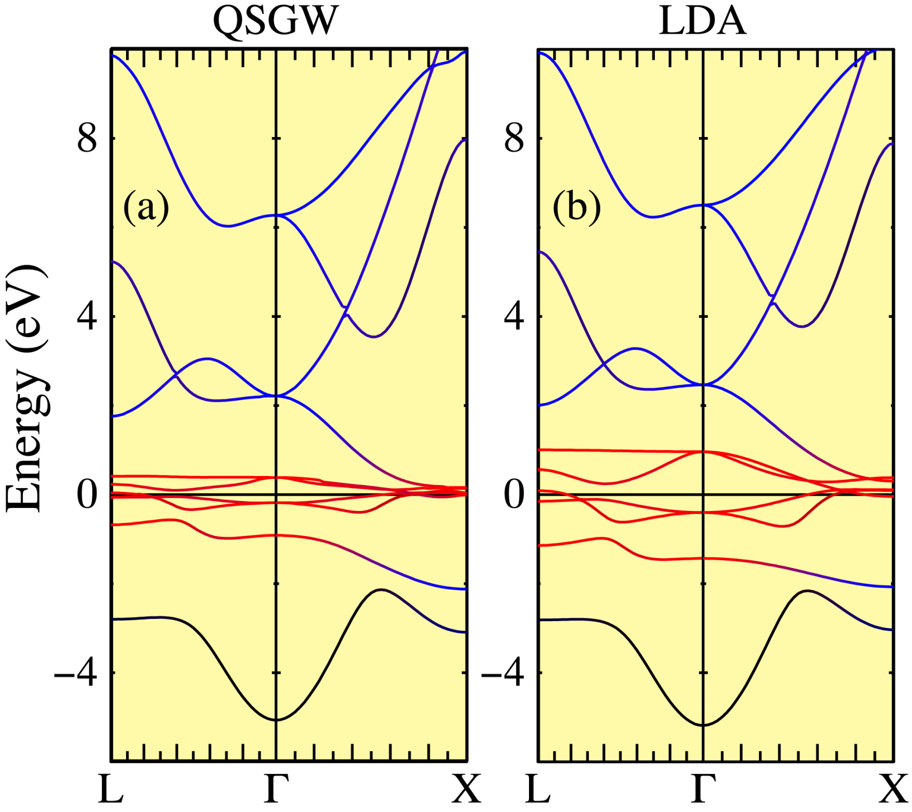

Figure 4-6 Electronic energy band structure of δ- plutonium, calculated by conventional Local Density Approximation (LDA) and the Quasiparticle Self-consistent Green's function Interaction (QSGW) methods [6]. The bands near the Fermi level (E ~ 0) are noticeably flattened in QSGW, showing, for the first time, electronic correlation effects from first principles electronic structure description of plutonium. Source: R. C. Albers, Los Alamos National Laboratory.

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Chapter 5: Panel 3 — Carbon Sequestration
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I. EXECUTIVE SUMMARY

Fossil fuels play an enormous role in our nation's base-load energy supply and provide reliable domestic energy security. Yet, if fossil fuels are to remain a component of energy production, amidst a worldwide call to reduce carbon dioxide (CO_2) emissions, then carbon-neutral energy options must be available. With fossil fuels, point-source environmental control technologies will be required to help comply with future CO_2 emissions standards. Carbon capture and storage consists of the separation of CO_2 from fossil fuels or flue gas, pipeline transport, and injection into deep geologic formations. Carbon sequestration technologies capture and store CO_2 that would otherwise reside in the atmosphere for long periods of time. Our current knowledge of the science and technology of sequestration strongly supports the use of geologic formations for the safe and permanent sequestration of captured CO_2. The United States has the diverse and large-capacity geologic formations (sinks) needed to validate commercial-scale sequestration. These sinks include saline reservoirs, coal seams, basalts, and mature oil and gas fields.

Deployment issues (including developing a regulatory framework, overcoming legal obstacles, and addressing operational concerns) can be directly addressed through the development of protocols advised by basic science research. The basic science gaps addressed in the three priority research directions (PRDs) identified in this report appear to be resolvable by means of laboratory and pilot-scale research supported with field applications. These PRDs include extracting high resolution information from subsurface imaging and modeling, understanding multi-scale dynamics of flow and plume migration, and developing the control science and tools needed to handle very low rate processes. The next decade will witness field validation and demonstration of carbon sequestration. This phase offers a test bed opportunity for basic science experimentation.

Carbon capture, a closely related technology, was the subject of two recent workshops — *Technology and Applied R&D Needs for Carbon Capture: Beyond 2020* and *Carbon Capture: Beyond 2010*. Details concerning carbon capture can be found there and are not covered in this chapter.

II. PANEL REPORT

Role of Topic in National Energy Picture

Carbon capture and sequestration consist of the sequence of steps shown in Fig. 5-1, culminating in the injection of CO_2 into a porous subsurface formation capped by a nonporous formation, which helps to permanently trap the spreading CO_2 plume shown schematically by the blue arrows. After CO_2 is captured from a power plant or other industrial source, it is compressed, transported, and injected through wells into deep geologic formations. An example of an injection well being drilled for a DOE pilot research project is shown in Fig. 5-2.

Multiple studies have shown that carbon capture and sequestration are a major element for mitigating climate change (for example, see Fig. 5-3). Carbon capture and sequestration technologies would allow the United States to (1) meet international greenhouse gas (GHG) reduction goals; (2) preserve the low cost energy that fossil fuels provide, supporting the high standard of living U.S. citizens have come to expect; (3) preserve the massive domestic investment in power-generating and industrial assets; (4) maintain energy security through a greater diversity of fuel options and exploitation of the abundant domestic fuel resources in the U.S.; and (5) provide a low-cost and reliable option for base-load electric power generation. Rapid commercial development and deployment of carbon capture and sequestration will help position the United States as a leader in the global clean energy race. Here, we focus on the sequestration part of the carbon capture and sequestration process.

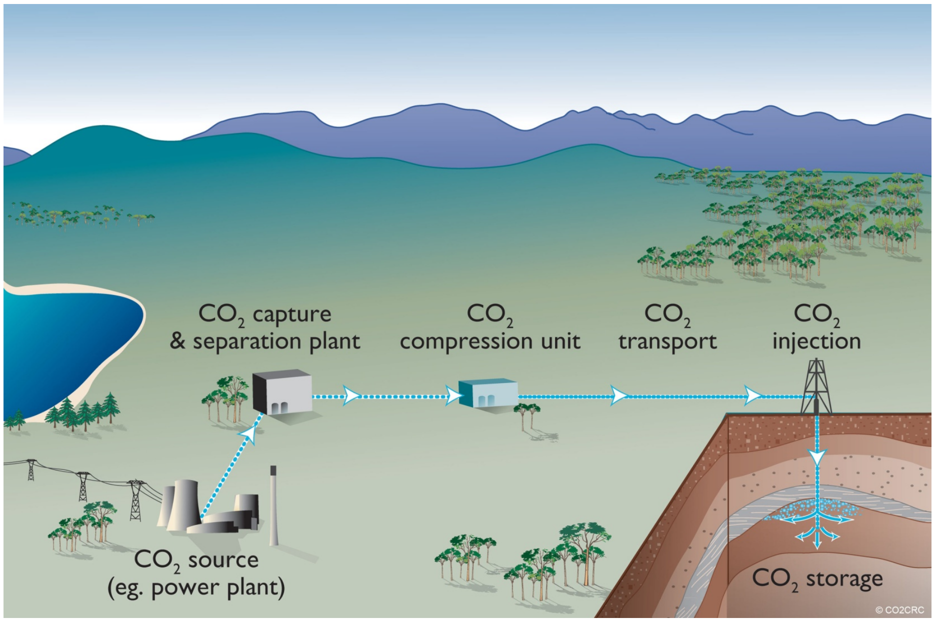


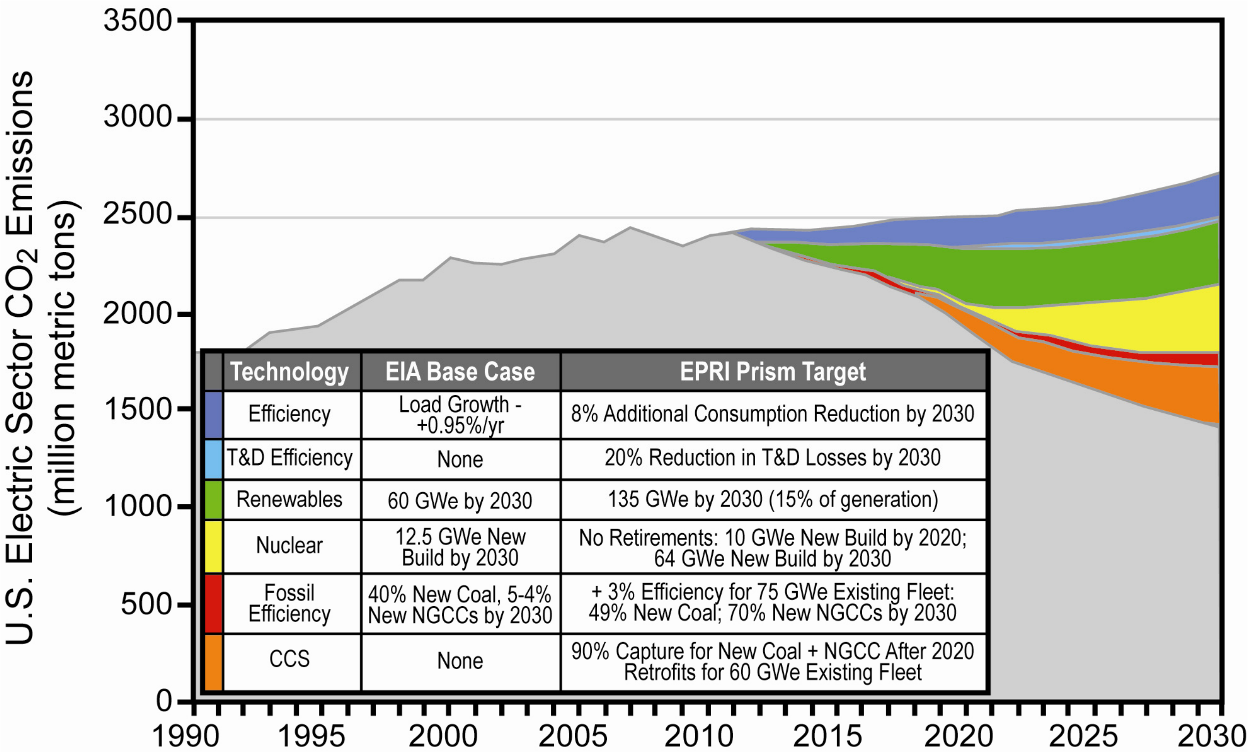
Figure 5-1 Schematic of carbon capture and sequestration. Source: Cooperative Research Centre for Greenhouse Gas Technologies (CO2CRC).

Status of Present and Ultimate Industrial Technology Deployment

The existing large base of experience, knowledge, and methods and tools available in other industries (e.g., oil and gas production, gas storage, and waste water disposal) can be applied to the geologic storage of carbon. Also applicable is the extensive knowledge of geologic formation properties and "cap rock" security for some specific locations, providing near-term opportunities for deployment of geologic sequestration technology. For other locations and rock types, many unanswered questions remain.

Technologies for carbon capture have reached the stage of prototype demonstration, and initial trials of geologic carbon sequestration have been completed. Nonetheless, the vast potential of this technology is just beginning to be tapped; ultimately, carbon sequestration can become one of the dominant methods for alleviating concerns about GHG and ensuring optimal use of our enormous fossil fuel resources. To realize this potential, major breakthroughs are required in basic science understanding, as well as in technology development and commercial-scale demonstration. Given the scale of sequestration needed to mitigate climate change and the short time frame required for GHG stabilization at acceptable levels, the basic science needs for this energy-related technology should be pursued with urgency.

Figure 5-2 Typical drilling operations of a CO_2 injection well. Source: R. A. Esposito, Southern Company.



	Technology	EIA Base Case	EPRI Prism Target
🟦	Efficiency	Load Growth - +0.95%/yr	8% Additional Consumption Reduction by 2030
🟦	T&D Efficiency	None	20% Reduction in T&D Losses by 2030
🟩	Renewables	60 GWe by 2030	135 GWe by 2030 (15% of generation)
🟨	Nuclear	12.5 GWe New Build by 2030	No Retirements: 10 GWe New Build by 2020; 64 GWe New Build by 2030
🟥	Fossil Efficiency	40% New Coal, 5-4% New NGCCs by 2030	+ 3% Efficiency for 75 GWe Existing Fleet: 49% New Coal; 70% New NGCCs by 2030
🟧	CCS	None	90% Capture for New Coal + NGCC After 2020 Retrofits for 60 GWe Existing Fleet

Figure 5-3 2009 PRISM analysis showing role that carbon capture and sequestration can play in reducing U.S. electric sector CO_2 emissions. Source: Electric Power Research Institute [1].

Context/Background for the Three Priority Research Directions

The total pore volume under the earth's surface at depths from one kilometer (where pressure and temperature permit CO_2 storage as a dense supercritical fluid) to five kilometers (where costs of installing wells are prohibitive) is immense. This condition speaks to the great promise of geologic carbon sequestration. There are also significant challenges to deployment, most of which relate to the uncertainty about site-specific geology. The uncertainty stems from the inherent variation in rock types, depositional environments, and reservoir properties, as well as the cost, resolution, and availability of geologic data that must be acquired at a depth where such information cannot be easily obtained. For example, innate geologic heterogeneity occurs from one location to the next because of spatial variation in past depositional environments in which reservoir rocks were formed. The uncertainty in reservoir rock parameters (porosity, permeability, thickness of the formation, existence of inter-bedded rock, etc.) leads to uncertainty in the model predictions used to assess the subsurface flow and transport of CO_2, displaced brine, and other constituents. Deformation in the subsurface long after deposition can lead to folds, faults, and fractures in the reservoir rock or the impermeable cap rock that is relied upon to seal the reservoir.

Tools exist to gather subsurface information such as seismic methods, resistivity, etc., but most of these techniques entail essentially subsurface remote sensing through a large overburden of rock. This remote sensing causes considerable energy loss in the signals, thereby significantly limiting the depth of penetration and method resolution. Higher resolution can be obtained by lowering sensing tools into the wellbore ("wire line"), but these tools provide data only in the immediate vicinity of the well. Very precise (and even more localized) information can be obtained from cores extracted during drilling of wells (Fig. 5-4). Both wire line sensing and core extraction come at significant cost, discouraging large-scale, high-resolution data collection. Wells with wire line logs and cores cost typically \$500,000 to \$3,000,000, depending on depth, amount of core, number of logs, etc.

Figure 5-4 Drill cuttings and whole core collected for site characterization of geologic sequestration. Source: R. A. Esposito, Southern Company.

The resulting sparse and imprecise information available today has caused the significant uncertainty mentioned above with regard to the 3-5 MMT/yr volumetric scale of a sequestration site, especially given the highly localized spatial heterogeneity of rocks. Further challenges exist when one considers the range of spatial and temporal scales. Some sequestered CO_2 instantly forms carbonic acid when dissolved in subsurface brine, resulting in the potential for mineral precipitation or dissolution. That induced geochemistry can take centuries to millennia to complete. Reactions taking place on the molecular scale may affect pore space and volume and, hence, multiphase fluid flow at the reservoir (10 km) scale. Thus, relevant spatial scales vary by ~15 orders of magnitude, and it is desirable to extrapolate temporal information covering a millennium from practical laboratory experiments.

Use of indirect methods of measurements, limited access to the subsurface environment, need for remote and noninvasive techniques, and heterogeneous geologic systems make it difficult to characterize and predict fluid flow through deep geologic reservoirs. Basic research is needed to gain a better understanding of flow and transport mechanisms and to develop instrumentation, modeling techniques, and monitoring tools that reduce uncertainty and ensure safe, reliable storage of CO_2. The carbon sequestration industry must be able to evaluate the safety of geologic storage, and reliable basic science can result in tools and methods to reduce this uncertainty.

Brief Description of PRDs

The Workshop panel identified three PRDs in which science can play a significant role supporting the technology development and commercial deployment of geologic carbon sequestration. These research directions are as follows: (1) extract high resolution information from subsurface imaging and modeling, (2) model the multiscale dynamics of flow and plume migration, and (3) develop the control science and tools to handle very low rate processes.

PRD#1: High Resolution Information. High resolution information from subsurface imaging and modeling would support a storage operator's ability to characterize the subsurface environment and monitor the movement of CO_2 and brine at the desired depth. This characterization is currently limited to borehole-based studies and low-resolution geophysical techniques. Geophysical methods will likely play an important role in site characterization, monitoring, and closure of geologic CO_2 storage sites. However, cost-effective, high-accuracy, and high-resolution geophysical methods are not available to measure deep formation properties and CO_2 saturation, to detect and quantify leakage of CO_2 and brine, or to account for the mass of CO_2 injected. Therefore, new or improved geophysical data collection, processing, inversion, and interpretation techniques are needed to ensure safe, commercial-scale deployment of CO_2 storage in deep reservoirs. Development of such techniques requires great advances in fundamental science understanding.

PRD#2: Multiscale Dynamics. The multiscale dynamics of flow and plume migration must be better understood to assess the long-term performance and safety of a CO_2 storage site in terms of capacity, injectivity, and containment. Methodologies and tools are needed to upgrade storage site properties from the pore to field scale and take into consideration rare or small-scale features that could significantly affect the storage integrity. Storage site operators must be able to accurately predict the pressure distribution from detailed characterization of the formation structure and physical properties of the subsurface, in particular, heterogeneities and no-flow boundaries. A viable large-scale geological model must include all components of a storage site at a level of detail where all key features are taken into account.

PRD#3: Control Science for Low-Rate Processes. Safe and permanent geologic sequestration requires methods for enabling experiments of short timescale to predict millennium-scale rate processes. Relevant geochemistry initiated by CO_2 injected into the subsurface can take thousands of years to complete. Climate models indicate that storage security must be high over the time span of future fossil fuel use to effectively mitigate climate change. Storage operations, tied to the lifetime of industrial facilities such as power generation, cement and steel manufacture, ethanol production, etc. are typically on the order of 40-70 years. At present, specific information about CO_2 behavior in a geologic formation can only be generated in the laboratory by using cores and brine extracted from wells and, pragmatically, in experiments with duration of days to months. A fundamental challenge is to generate accurate, long-term predictions of low-rate processes by experimental methods that are shorter by two to five orders of magnitude. In order to understand the ultimate fate of geologically sequestered CO_2, long-term flow and mineral trapping processes must be understood well enough to be able to generate accurate parameters for predictive models. The ability to predict and model these processes can greatly aid in resolving liability, regulation, insurability, and other pragmatic issues that could strongly impact the viability of this option for mitigating climate change. The challenge is one of basic science: how can long-term rate processes be reliably predicted from short-term data?

The previous Basic Energy Sciences Workshop on Basic Research Needs for Geosciences (February 21–23, 2007) identified several PRDs that have common elements to those described herein: (1) dynamic imaging of flow and transport and (2) determination of transport properties and in situ characterization of fluid trapping, isolation, and immobilization. These two sets of PRDs differ from each other in that this report places emphasis on improving the geophysical approaches used to image CO_2 plume position in the deep subsurface, greatly expanding the spatial resolution of reservoir properties used in models to predict CO_2 transport and evaluating and predicting geochemical changes to CO_2-contacted reservoir rock and well materials that operate over long timescales. Both sets of priority research directions share the fundamental objectives of improving existing methods or developing new approaches for monitoring and predicting fluid movement in the subsurface, which are needed for safe, reliable CO_2 storage.

III. PRIORITY RESEARCH DIRECTIONS

A. PRD #1: Extracting High Resolution Information from Subsurface Imaging and Modeling

1. Problem Statement

Our ability to characterize the subsurface environment and monitor the movement of CO_2 and brine within the earth to depths below 10,000 ft is currently limited to borehole-based measurements and geophysical techniques that have variable spatial prediction sensitivity. Borehole-based observations are highly effective for characterizing small-scale formation properties, but a dense network of expensive wells may be needed to collect large enough statistical samples to quantify uncertainties to an acceptable level for accurate prediction to adequately characterize formation heterogeneity, which controls fluid movement and its distribution in the subsurface. Selecting the optimum location of each well for monitoring purposes is difficult because spatial heterogeneity can result in discrete fast-flow pathways, making it difficult to predict a priori where a well should be placed to best detect CO_2. Geophysical methods (seismicity, electrical resistivity, gravity, etc.) have proven that they can predict many of these subsurface parameters adequately in the process of hydrocarbon extraction (see Fig. 5-5). These same tools and methods hold great promise for delivering this same level of dependability for remotely characterizing formation properties on a larger scale, and for detecting and monitoring CO_2 movement associated with many types of heterogeneous geologic storage formations. The combination of these factors to interpret processes can dependably be used for selecting monitoring well locations. However, additional research is needed to validate and/or improve the reliability, resolution, and accuracy of these remote sensing methods. This research would provide greater confidence that the methods can be deployed to accurately characterize a geologic storage site and safely monitor large-scale CO_2 injection projects. Integration of geophysical data with conventional well-bore data that are tightly integrated with the broad knowledge about geologic reservoirs in the subsurface is required for accurate construction of reservoir models that can be used to constrain CO_2 (and brine) interactions. These data can also be used in the reservoir simulation transport model to predict the overall subsurface impact of CO_2 injection.

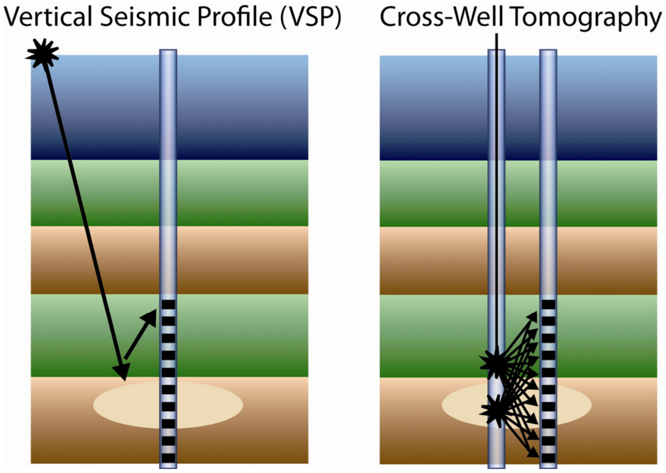


Figure 5-5 Promising geophysical techniques. Vertical seismic profiling and cross-well seismic surveys are used to create subsurface images. Source: D. Peters, Schlumberger Carbon Services (presented at 2009 SECARB annual meeting).

2. Executive Summary

Geophysical techniques are commonly used to prospect for oil, natural gas, and mineral deposits. Geophysical methods will play an important role in site characterization, monitoring, and the closure of geologic CO_2 storage sites. However, cost-effective, high-accuracy, and high-resolution geophysical methods are needed by industry to measure deep formation properties and CO_2 saturation, detect and quantify leakage of CO_2 and brine, account for the mass of CO_2 injected, and comply with future regulations. Therefore, new or improved collection, processing, inversion, and interpretation techniques for geophysical data are needed to facilitate safe, commercial-scale deployment of CO_2 storage in deep reservoirs. Furthermore, methods for combining geophysical data with conventional reservoir data are needed to build CO_2 transport models and constrain the results from such models.

3. Industry Need

The U.S. Environmental Protection Agency (EPA) was granted authority under the Safe Drinking Water Act to promulgate rules that regulate the injection of fluids into the subsurface to protect underground sources of drinking water (i.e., groundwater). The EPA created the Underground Injection Control (UIC) program to administer and enforce the rules. In 2008, the EPA proposed draft UIC rules that would regulate the underground injection of CO_2 for geologic storage purposes. The new draft Class VI well standard requires that the project proponent characterize the nature and extent of the high-permeability, high-porosity injection reservoir(s) used to store the CO_2 and the low-permeability confining unit(s) used to safely contain the CO_2 underground. In addition, the project proponent must monitor the extent of the pressure and CO_2 fronts throughout the injection and post-injection closure period to ensure that CO_2 does not leak from the storage reservoir. Techniques that provide high quality images of the fluid saturations in the subsurface can be used to optimize injection operations, taking maximum advantage of available pore space and allowing for the accounting of stored CO_2 under a future carbon cap and trade economic program. For regulatory compliance and storage optimization, high-resolution geophysical techniques are needed to characterize in detail the heterogeneous distribution of formations and formation properties and to accurately track brine leakage and CO_2 plume dimensions, saturations, fronts, and fast-flow pathways (see Fig. 5-6). Borehole or surface-based geophysical techniques that detect CO_2 dissolved in groundwater are also needed because the dissolved CO_2 front often precedes the arrival of the free-phase CO_2, thus serving as an early warning indicator of CO_2 arrival or leakage.

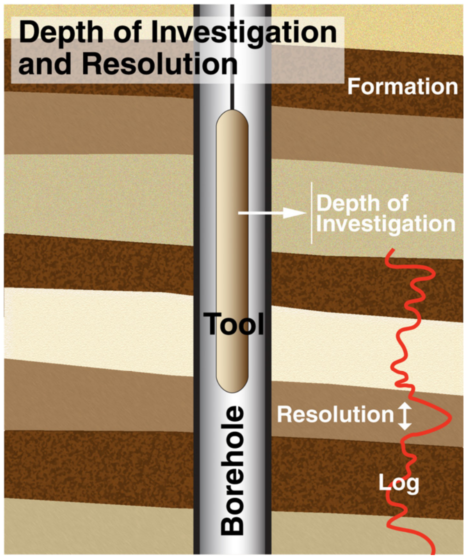


Figure 5-6 Schematic illustrating depth of investigation and resolution for a borehole-based geophysical logging tool. Improved methods for imaging deep reservoirs from the land surface are also needed. Source: D. Peters, Schlumberger Carbon Services (presented at the 2009 SECARB annual business meeting).

4. Scientific Challenges

The immense volume of CO_2 required to be sequestered from industrial sources to reduce global climate change will require widespread deployment. Given the immense volume of CO_2 that could be injected, accurate accounting of the CO_2 mass retained in the subsurface will be required to demonstrate compliance with EPA environmental standards and to prevent forfeiture of carbon credits from unaccounted CO_2, should a mandatory carbon cap and trade system be implemented. Geophysical methods with high accuracy and resolution could play a significant role in detecting leakage and accrediting geologic storage projects. Quantifying and improving the accuracy, resolution, and reliability of geophysical measurements over a broad range of formation types, reservoir depths, areas, and volumes will be challenging, not only for detecting leakage to protect public health, safety, and property, but also for determining project feasibility and sequestration economics. Making higher resolution geophysical measurements at greater depths and over larger volumes, improving data inversion techniques, and improving methods for combining geophysical with non-geophysical data sets to constrain and improve the accuracy of the overall results are some of the scientific challenges that need to be addressed.

5. Research Directions

Key research directions that will promote the deployment of sequestration at a commercial scale include the following:

- New methods of subsurface imaging, data processing, and interpretation at great depths and over large areas for both characterization and monitoring purposes. A specific area of interest is predicting pressure fronts over large distances that may only be affected by small changes and verifying that the effect of the pressure front is from CO_2 injection and not some other background response. Most geophysical tools can sense pressure changes to varying degrees near the wellbore or in wellbore sensors and are accurate, but can this near-bore knowledge be adequately employed for monitoring the CO_2 effect far away from the injection site? Surface seismic data can sense pressure changes, but what accuracy is needed to validate CO_2 injection changes?

- Investigation of the effect on the seismic response as the CO_2 saturation changes in the brine and determination of whether this effect can be detected when in a supercritical liquid phase vs. a gas phase. The hope is that CO_2 will stay in the liquid phase, but it would potentially be more detectable by surface seismic testing in the gas phase by using the AVO (amplitude versus offset) technique, much like natural gas. This method is commonly referred to as "bright spot" detection in the oil and gas industry. Further research will correlate the theoretical response to actual seismic response in an operational injection site and, most importantly, validate measurements and models over time and the space actually covered by the CO_2 plume.

- Integration of geophysical measurements into reservoir simulators to help constrain flow and transport predictions. This task will begin to establish the boundaries of the CO_2 migration inclusive of the anticipated error in the modeled result. The measurement sensitivity and calibration within and between observation of wells away from the main injection site need to be investigated.

- Development of rock-physics models or transform functions to derive formation and/or fluid properties (especially permeability, porosity, and CO_2 saturation) from geophysical data in the presence of CO_2 in its multiple phases and at pressures as seen over time. In particular, the role of standard core analysis procedures in defining these critical rock physics parameters at the wellbore and their extension to the geophysical responses need to be studied: Are the current techniques adequate or are new techniques needed?

- Determination of what effect the long-term geochemistry has on the formation petrophysics, and how geophysics can be used to image and evaluate these effects to inform and optimize storage operations. These need to be built into robust models that define the location of injected CO_2 and predict its movement over time, inclusive of the uncertainty in the model.

6. Potential Impact

A high resolution set of geophysical tools that can be used to reliably image CO_2 and brine movement in the subsurface is critical to fostering a major national program of carbon sequestration, which for decades to come will be the largest single method of reducing greenhouse gases (see Fig. 5-7). More specifically, this set of tools would provide a number of potential benefits:

- A proven monitoring tool that can be used to comply with proposed EPA regulations governing geologic storage of CO_2;

- An improved site characterization tool that industry can rely on to provide increased confidence that a sequestration project will be safe and economically feasible prior to incurring large capital expenditures for capture equipment and obtaining injection permits;

- Increased confidence in the long-term outcome that storage will be safe and secure, allowing industry to obtain the financial backing needed for large-scale projects to be deployed and to reduce investor concerns over long-term liability;

- A much needed method for validating the permanence of CO_2 storage and accrediting storage projects for credits, if a carbon cap and trade program becomes mandatory in the future.

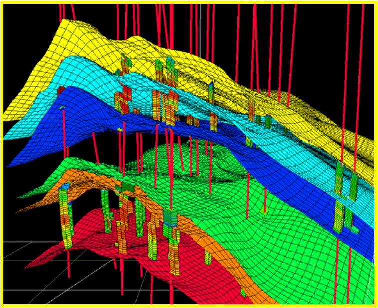


Figure 5-7 Combined geophysical data with conventional reservoir data. This information can be used to create robust static and dynamic 3D geological models (pictured) and constrain fluid flow models used for CO_2 transport. Scale: approximately 2 miles in the vertical direction, and approximately 3 miles in each of the horizontal directions. Source: D. Peters, Schlumberger Carbon Services (presented at the 2009 SECARB annual business meeting).

B. PRD #2: Understanding Multiscale Dynamics of Flow and Plume Migration

1. Problem Statement

Inadequate model construction and implementation could lead to false representation of risk associated with CO_2 storage projects, both before and after injection operations begin. To accurately model CO_2 migration in the subsurface, site characterization measurements carried out at vastly different scales will need to be integrated to populate the geological model with properties that are relevant to predicting CO_2 flow. Further, these properties will need to be scaled up without removing small-scale features that could have a significant effect on simulating CO_2 flow and plume migration. The modeling process must be coupled to proper monitoring and measurement techniques in the field.

2. Executive Summary

Understanding flow dynamics at different spatial dimensions and timescales is essential to properly assess the performance characteristics of a CO_2 storage site in terms of capacity, injectivity, and containment (see Fig. 5-8). While capacity and injectivity drive investments and operational costs, containment relates directly to safety, more precisely to the safeguarding of populations and the environment against possible leakage due to loss of storage integrity. To

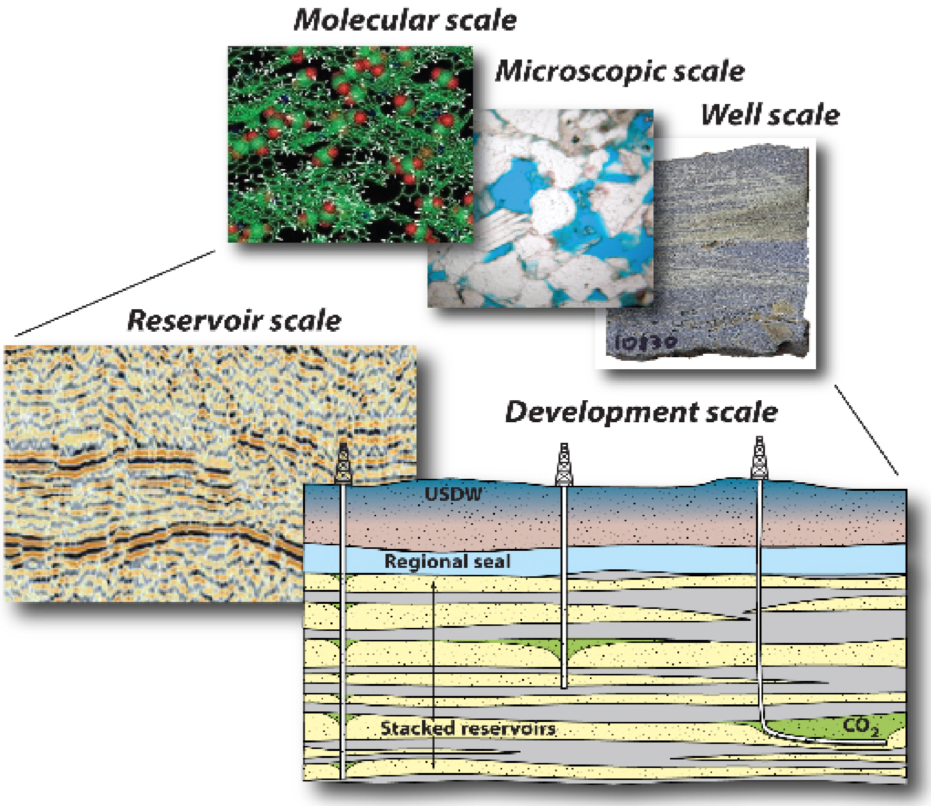


Figure 5-8 Drawings illustrating spatial behavior of CO_2 at various scales to accurately assess storage performance. Source: J. Pashin, Geological Survey of Alabama.

accurately quantify risk associated with underground CO_2 storage projects, the following advances are needed to develop methods to upgrade pore-scale properties to field-scale models, determine the effect of a pressure increase on rock integrity, simulate scenarios of plume migration after loss of containment, and establish proper monitoring protocols to validate model predictions. These advances require fundamental science understanding.

3. Industry Needs

Capacity, injectivity, and containment are assessed with increasing accuracy as a CO_2 storage project matures, i.e., advances from exploration and site selection to appraisal. Associated risks are also evaluated in terms of probability and impact by using first qualitative then more quantitative approaches. Such studies rely heavily on measurement campaigns and modeling studies, complemented by injection tests and pilot projects at a later stage. Key performance indicators include pressure distribution, the effect of overpressure on underground formations, brine displacement in the reservoir and eventually in the whole aquifer system, CO_2 plume lateral extension and possible migration out of the storage formation, leakage scenarios, and risk criticality, all of which have associated uncertainties.

After a "go" decision is reached, the storage site will be further developed. This phase will increase significantly the level of investments. In particular, well/field design and storage optimization plans leading to a "go" decision will have to be based on models, based upon a level of detail of the subsurface structure and properties, that enable accurate predictions of the injection and fate of the CO_2. The industry need is to focus on developing and establishing these models, which pose significant scientific challenges as described in the next section.

4. Scientific Challenges

The injection in the subsurface of CO_2 will immediately translate into an overpressurization of the formation fluids, with possible effects on the movement of native fluids or the mechanical stability of the rock. A CO_2 plume will form. This plume will evolve depending on the injection pattern, the structural and depositional characteristics, and the underground formation's physical properties (see Fig. 5-9). Both pressure and CO_2 plume evolution must be carefully characterized to avoid adverse effects on safety and storage efficiency. This characterization is achieved by first building a detailed descriptive geologic model of the storage site, which represents the structure of underground formations and their properties, including all components: reservoir, cap rock(s) and overburden, faults, and wells.

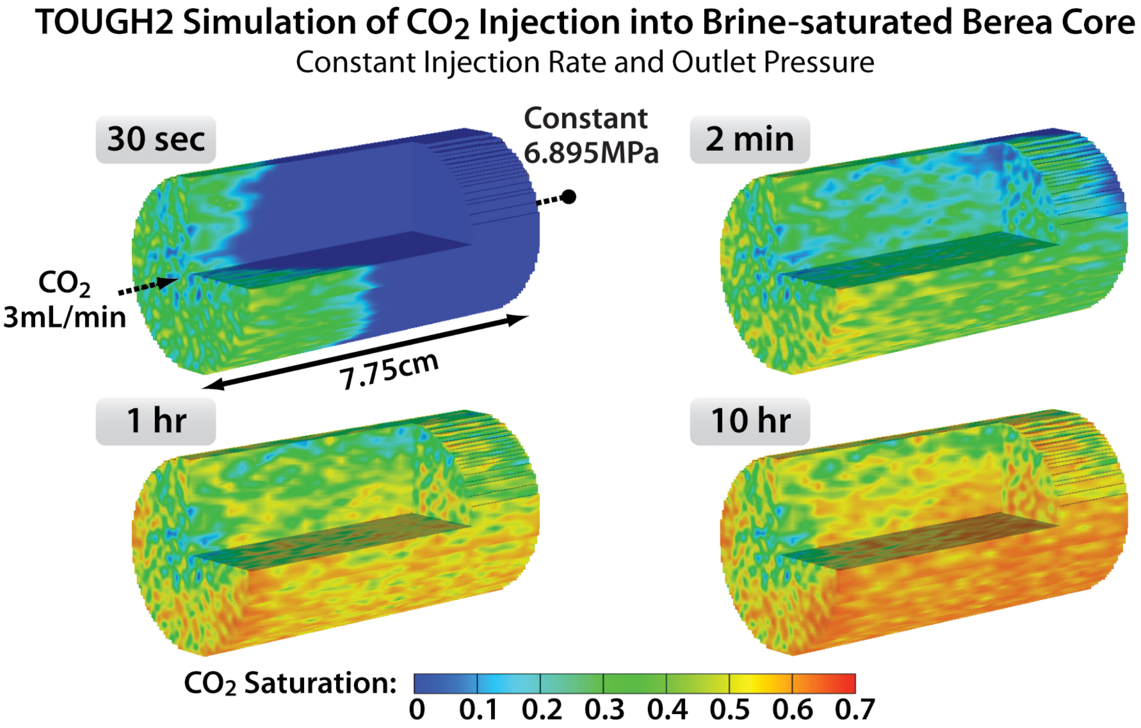


Figure 5-9 Simulation of CO_2 injection into brine-saturated core over 10-hr period. Since heterogeneity controls CO_2 saturation, understanding the physical properties and causes of heterogeneity in rocks is key to the prediction of CO_2 movement in the subsurface environment. Source: S. Benson, Stanford University.

Formation heterogeneity is inherent in all geologic systems because of the natural spatial variation in terrestrial, fluvial, and marine environments in which sediments are deposited, eroded, and re-worked over time. In turn, formation heterogeneity plays an important role in controlling the spatial distribution of injected fluids underground.

Faults, folds, and fractures resulting from regional tectonics will add structural complexity and overlay additional heterogeneity onto a sedimentary system. In the case of CO_2 injection, they will translate into different conditions (permeability distributions and flow boundary conditions) for the over-pressure to propagate and the CO_2 plume to evolve. Furthermore, regional hydrodynamics must be understood to evaluate the risk of displacing native brines. The continuity of the primary cap rock should be assessed too, with the detection of fast-flow pathways such as faults or intrusion of sand bodies that bypass the seal (see Fig. 5-10). The challenge is to capture all the relevant features and variations of properties of large geological systems, relying upon a limited amount of data, such that CO_2 movement can be accurately forecast by means of reservoir simulators. Often, the availability of data is driven by economic considerations as well as technological ones.

Property modeling can be used to complement this large-scale identification of geologic structures and stratigraphic sequences. It would consist of integrating estimations of physical properties such as porosity, permeability, elastic moduli, rock strength, and in situ stresses, which are performed at various scales (core, log, or even coarser when obtained from well tests or seismic surveys). Geostatistics must be used to extrapolate wellbore data to the entire 3D volume of interest. The scientific issue is to integrate characterization measurements carried out

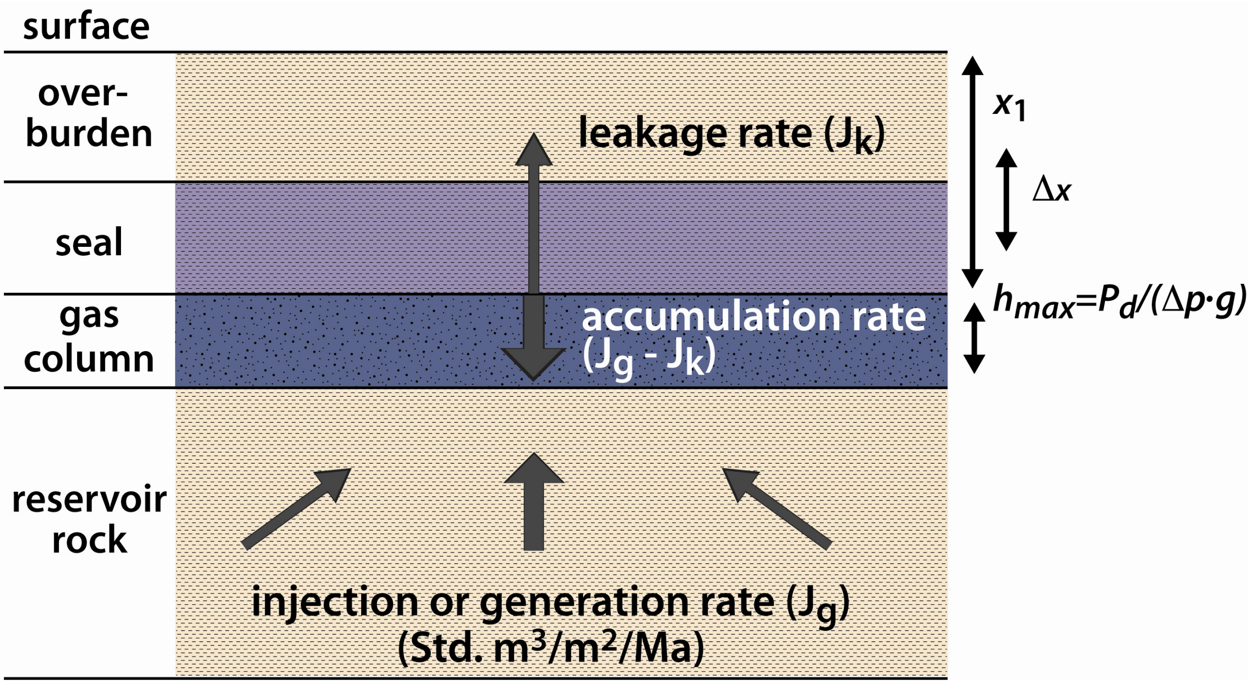


Figure 5-10 Model showing the effects of heterogeneity across cap rocks and the relationship of cap rocks with target formation. Source: [2].

at vastly different scales to populate the geological model with properties that are relevant to CO_2 flow and to upgrade the scale of these properties without removing small-scale features that could have a significant effect (e.g., a thin layer with low permeability that could act as a flow barrier or with low strength property that could fail with increasing pore pressure). The inherent disorder and nonlinear behavior of materials are aspects that can be addressed by bringing to bear state-of-the-art physical theory and advancing it.

Dynamic simulation of CO_2 injection would follow property modeling. Modeling frameworks have already been developed to account for key processes such as multiphase flow, geochemistry, geomechanics, and heat transfer. Numerous studies are ongoing to couple these processes in the context of CO_2 storage. Simplified models have already been run for existing storage projects, after proper calibration with laboratory and field data, and are being progressively refined to properly account for monitoring observations. However, scientific gaps still remain in the determination of the required level of coupling for these processes and on the representation of heterogeneities. Detailed models are required for modeling short-term near-wellbore phenomena that may affect injectivity (precipitation or dissolution of solids). Furthermore, fully coupled models at the microscopic level, properly calibrated with core experiments, are required to compute effective parameters to be input in reservoir simulators. However, a high level of detail – both in terms of resolution and physical processes – may not be practical for large-scale simulations, in particular, for the evaluation of long-term processes occurring in the whole storage reservoir (e.g., mineralization). Whatever level of detail is incorporated in the model, its predictions will need to be calibrated and validated by comparing model results to monitoring measurements. There are significant scientific challenges at each of the tasks described above.

5. Research Directions

- Developing methodologies and tools to scale properties from the pore up to the field scale, while keeping rare or small-scale features that could significantly affect the pressure distribution and the displacement of fluids. Such scaling should use sensitivity analysis considering physical processes such as fluid dynamics and geomechanics.

- Determining the effect of CO_2 injection on in situ rock stresses, resulting in potential fluid-pressure-induced seismicity and fault reactivation. Predicting accurately the pressure distribution requires a detailed characterization of the subsurface – formation structure and physical properties – in particular, heterogeneities and no-flow boundaries. Such a requirement emphasizes the need for a proper large-scale geological model that includes all components of a storage site at a level of detail where key features are taken into account.

- Accurately predicting the CO_2 plume displacement and fate in the storage formation, including possible plume migration scenarios in case of losses of containment. Such models will have to account for all features that influence plume displacement, for instance, natural heterogeneities of the geological media but also physical phenomena such as trapping mechanisms (e.g., dissolution or mineralization), all occurring at multiple scales.

- Proper monitoring protocols and history-matching techniques for model calibration, in particular, pressure and CO_2 saturation distribution. Here, the difficulty will be to quantify the confidence in long-term predictions from models calibrated on measurements taken over a limited time.

6. Potential Impact

Solving the scientific challenges associated with the multi-scale dynamics of flow and plume migration will increase industry's ability to accurately model the CO_2 plume behavior and assess the potential impact of its migration. Success with the above research directions will strongly improve the deployment of the CO_2 storage technology: adequate solution of these key challenges will provide tools to better assess the early stages of the storage site lifecycle, improve the site operation, provide adequate support for regulatory compliance, and provide the basis for adequate monitoring of the CO_2 fate at all times. Ultimately, long-term plume prediction is a necessary element for a successful carbon sequestration program on the scale needed by our nation.

C. PRD #3: Control Science and Tools to Handle Very Low Rate Processes

1. Problem Statement

Relevant geochemistry initiated by CO_2 injected into the subsurface can take thousands of years to complete. Climate models indicate that storage security must be very high for over a thousand years to effectively mitigate climate change. Yet, specific information about CO_2 behavior in a geologic formation can only be generated in the laboratory by tests with cores and brine extracted from wells and, pragmatically, in experiments with duration of days to months. A fundamental challenge is to generate accurate, long-term predictions of low-rate processes by methods that measure on a timescale that is shorter by two to five orders of magnitude, and that will establish confidence in the security of the stored CO_2 on the timescale of commercial operations (see Fig. 5-11).

2. Executive Summary

There is a mismatch between the long timescales required to mitigate climate change and subsurface processes that may trap and immobilize the injected CO_2 vs. a realistic experimental timescale to research CO_2 behavior and the duration of commercial operations. Storage operations, tied to the lifetime of industrial facilities such as power generation, cement and steel manufacture, ethanol production, etc., are typically on the order of 40 to 70 years. As stated above, climate change mitigation requires storage security on the millennial timescale. Trapping mechanisms, which immobilize the CO_2 plume and can provide storage security, take decades to centuries for dissolution and capillary trapping and millennia for mineralization. Understanding

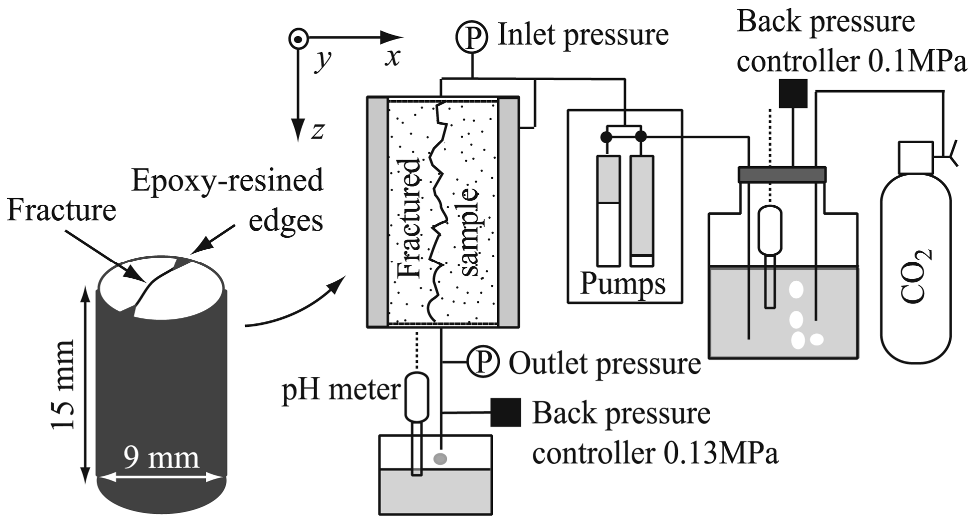


Figure 5-11 Laboratory instrumentation to accurately measure the pressure and flow systems of CO_2 brine and minerals in cap rocks. Results are used in the simulation of CO_2 chemistry for long timescales. Source: [3].

the ultimate fate of geologically sequestered CO_2 requires accurate parameters for predictive models. The ability to predict, model, and potentially control these processes can have a profound effect on liability, regulation, insurability, and other pragmatic issues that could strongly affect the viability of this option for mitigating climate change. The challenges for basic science are: How can long-term rate processes be reliably predicted from short-term data? Can these low-rate process timescales be manipulated via geochemical or biogeochemical methods? Control of trapping mechanism rates to accelerate them to the timescale of commercial operations is desirable, but at the same time, injectivity will typically need to be maintained for 50-70 years. For this reason, control science applied to this field requires tools that can provide accurate temporal extrapolation of physical and chemical phenomena, so that rates can be accelerated to an appropriate level to provide beneficial effects on storage security without having a deleterious effect on injectivity and emplacement of the CO_2.

3. Industry Need

Climate models indicate a need for urgent action with geologic carbon sequestration as one of the principal solutions, but confidence in geologic storage must extend for a thousand years or more. Additionally, capital investments in thermal plant infrastructure (large-scale industrial processes and power generation) are extremely large, requiring facilities to operate 40-70 years for a reasonable return on investment. Industry needs tools to provide greater confidence that a sequestration site will maintain operational viability (suitable injectivity) for a 50-year timescale and storage security for significantly longer. The ability to model and predict the onset of trapping mechanisms and plume stabilization (and perhaps even manipulate them) would benefit both industry and regulators.

4. Scientific Challenges

Detailed knowledge of subsurface geochemistry and other rate mechanisms associated with introduction of new chemical species is normally developed via laboratory experiments on extracted rock core and brine samples. In practice, the timescale of a laboratory experiment is limited from days to months. The challenge is to extrapolate the information gathered in the lab to in situ behavior over a much longer timescale. New experimental methods can measure chemical changes on an extremely small scale, but determining bulk changes over extended periods based on such data is not straightforward. New experimental, theoretical, and computational methods that can address this problem would be of broad interest to society because they would be applicable to engineered geologic systems, corrosion, materials degradation, and many other problems of economic and public safety importance. Additionally, these tools would facilitate studies of methods to manipulate long-term rates. Another issue is how to apply rate information gathered on small samples to larger scales in heterogeneous formations.

5. Research Directions

- Finding new approaches to handle temporal scaling is perhaps the largest and most pressing challenge. For example, to accurately predict plume stabilization, slow geochemical processes must be accurately modeled from relatively short-term experiments on core samples. Advanced analytical techniques, such as those provided by synchrotron X-ray sources, can provide the sensitivity and penetration to capture very early stage chemical changes in bulk, but extrapolation of the temporal behavior of these processes over many orders of magnitude remains a challenge. New experimental methods and designs as well as theory that can establish mechanisms and overall rate laws and orders from extremely early stage process data are needed.

- Understanding long-term geochemical effects on formation petrophysics, trapping, and injectivity. While geochemical products in high CO_2 environments may be predictable, dissolution/deposition rates, induced surface morphology changes, and other factors can affect the petrophysics of an underground formation. These factors, in turn, can affect injectivity in the operational phases of sequestration projects and trapping mechanisms as well. Formation chemistry, including structural changes in a complex environment such as heterogeneous porous media, must be understood.

- Employing geochemistry and/or biogeochemistry to accelerate plume stabilization and trapping mechanisms. The primary plume stabilization/trapping mechanisms are capillary trapping, solution trapping (brine with dissolved CO_2 is more dense and sinks), and mineral trapping. Introduction of chemical and/or microbial species may make it possible to manipulate these rates either for barrier formation or for general plume stabilization. For example, the carbonate/bicarbonate equilibrium can be shifted by some chemical species, which could accelerate solution trapping (see Fig. 5-12). Chemical and/or microbial species can accelerate mineral formation rates and might also produce surface modifications that affect capillary trapping. Because over-acceleration can be deleterious to operations, controlled processes are still long timescale, and the ability to accurately extrapolate and predict behavior as outlined in the first bullet may be critical to control science in this field.

- Understanding partitioning and transport of trace impurities and co-sequestration of chemical species, their geochemistry, and effects on materials. The primary question here is what purity of CO_2 is really required? Basic science can address issues such as what is the effect of trace impurities on material corrosion rates, and how those impurities might partition in the subsurface given the complicated multiphase flow and reactive transport. There could be cost savings in co-sequestering other gases that might be produced along with CO_2 in industrial processes of power generation. Improved understanding of this complex geochemistry would be desirable.

6. Potential Impact

Solving the scientific challenges associated with the research directions highlighted above will result in the development and calibration of new models, with an end result of increasing the confidence in the long-term outcome that geologic storage will be secure. Control science will be a key issue in obtaining regulatory approval and gaining overall public acceptance of geologic storage operations. This science will also allow for the optimum use of pore space for storage optimization and facilitate carbon sequestration on the vast scale needed to meet the world's climate needs.

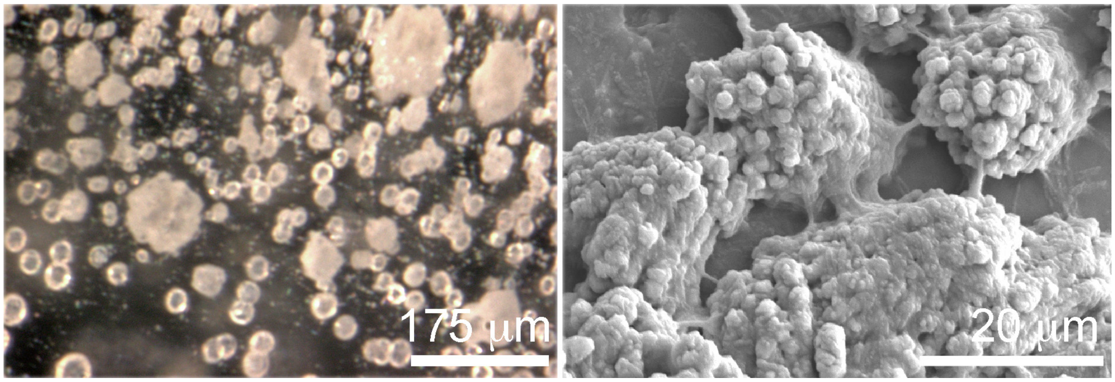


Figure 5-12 Calcite crystals formed at subsurface relevant pressure and temperature using a biomineralization process. Higher resolution (right) reveals the close association of microbes (cylinders) and crystallites (underlying structure). Source: L. Schultz, L. Wheeler, A. Mitchell, R. Gerlach, and A. Cunningham, Montana State University.

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Chapter 6: Panel 4 — Electrical Energy Storage
Coordinator: Bart Riley, A123 Systems

Panel Members:
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- Michael Everett, Maxwell Technologies
- Alan Gotcher, Gotcher & Co.
- Esther Takeuchi, SUNY-Buffalo
- Harshad Tataria, General Motors

I. EXECUTIVE SUMMARY

Electrical energy storage is critical to the nation's goals to reduce use of fossil fuels, reduce carbon dioxide (CO_2) and greenhouse gas emissions, and increase our energy security. Here, the focus is on electrochemical storage, including batteries and supercapacitors, particularly for transportation using plug-in electric vehicles and for utility-scale storage to meet issues arising from intermittency of renewable energy sources like solar and wind. Research and development (R&D) breakthroughs are needed that can offer the truly significant increases in performance at lower cost to meet national needs. This panel summary report identifies three science areas that would have the biggest impact in advancing the field of energy storage: new materials, novel architecture/processes, and understanding of interfaces. New materials are a key to improved performance at lower cost. New architecture or processes are also needed to go beyond incremental improvements in existing materials. Fundamental understanding of interfaces and the electrochemistry at those interfaces will accelerate the research into improved performance at a lowest cost.

II. PANEL REPORT

Role of Energy Storage in National Energy Picture

The importance of energy storage has grown over the past decades and has reached an unprecedented level as our nation electrifies transportation and integrates alternative energy, especially intermittent wind and solar energy, into our electrical utility grid, and as consumer use of portable, wireless electronic devices increases. Reduction of CO_2 emissions and the consequential reduction in global warming is now an international imperative, with nations around the world striving for leadership. Historically, leadership in energy storage technology and commercialization did not reside in the United States. However, the clear need for such technology has renewed interest in developing a domestic advanced battery industry. The need for energy storage technologies is being driven by potentially enormous market demands, yet there remain significant technical and economic challenges to widespread implementation.

Americans consume one-fourth of the oil produced globally, with transportation relying on petroleum for 94% of its delivered energy. The U.S. economy is critically dependent on oil, which makes it vulnerable to price volatility and disruptions in supply. Demand continues to grow, while suppliers are unable to increase production to keep up. Thus, we pay a high price in national security costs, as well as in constrained foreign policy, in order to maintain a reliable supply of petroleum. The environmental costs are also significant, with the transportation sector accounting for one-third of total CO_2 emissions in the United States. Finally, the trade imbalance, including $350 billion (B) per year to foreign oil producers, hurts the nation and undermines other foreign policy and humanitarian objectives.

Energy storage is playing a critical, growing role in the nation's transportation system. Quite simply, electrochemical storage technology in batteries and capacitors enables new vehicle architectures, like hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs), and all-electric vehicles (EVs.) These vehicles reduce or potentially eliminate the use of petroleum fuels. With the adoption of PHEVs and EVs, multiple sources of electricity including nuclear, hydroelectric, geothermal, wind, solar, and, for the time being at least, fossil energy, can be used to power our nation's vehicles. A greater diversity of energy sources will not only reduce our imports of foreign oil, it will make us less vulnerable to supply disruptions due to natural disasters and military, terrorist, or economic attack.

Energy storage also could have a critical impact in the way we generate, transmit, and distribute power through the nation's grid. Coal accounts for nearly half of the power generation in the United States. In order to achieve CO_2 reduction targets, we will need to develop renewable energy sources, such as wind and solar. However, intermittency of photovoltaic (PV) — solar and wind — creates a greater demand for ancillary services, such as frequency regulation, which allows grid operators to balance generation (supply) and load (demand) on short time scales, thus maintaining constant frequency and voltage. There has been concern that the nation's grid will not be able to handle more than 20% to 30% intermittent energy sources, such as renewables, due to the lack of sufficient ancillary services and fast-responding resources. Energy storage is expected to facilitate the greater penetration of renewables, by offering fast-responding services at competitive rates, while not contributing to emissions. In addition, energy storage allows timeshifting, where energy is temporarily stored for later release. Energy storage can similarly help wind developers firm their output and generate more revenue [1]. Energy storage can also lead to higher efficiency and utilization in the transmission system, while allowing existing assets to be used more effectively. Energy storage would also make the grid more robust to disruptions, thus increasing reliability and power quality. A hypothetical example of the effect of intermittency on the grid is shown in Fig. 6-1.

In summary, energy storage offers many benefits in grid and transportation applications, including:

1. Improved fuel utilization and reduced consumption of fossil fuels;
2. Reduced CO_2 and other greenhouse gas emissions;
3. A greater diversity of energy sources, increasing the nation's energy security and decreasing our dependence on foreign sources of energy;

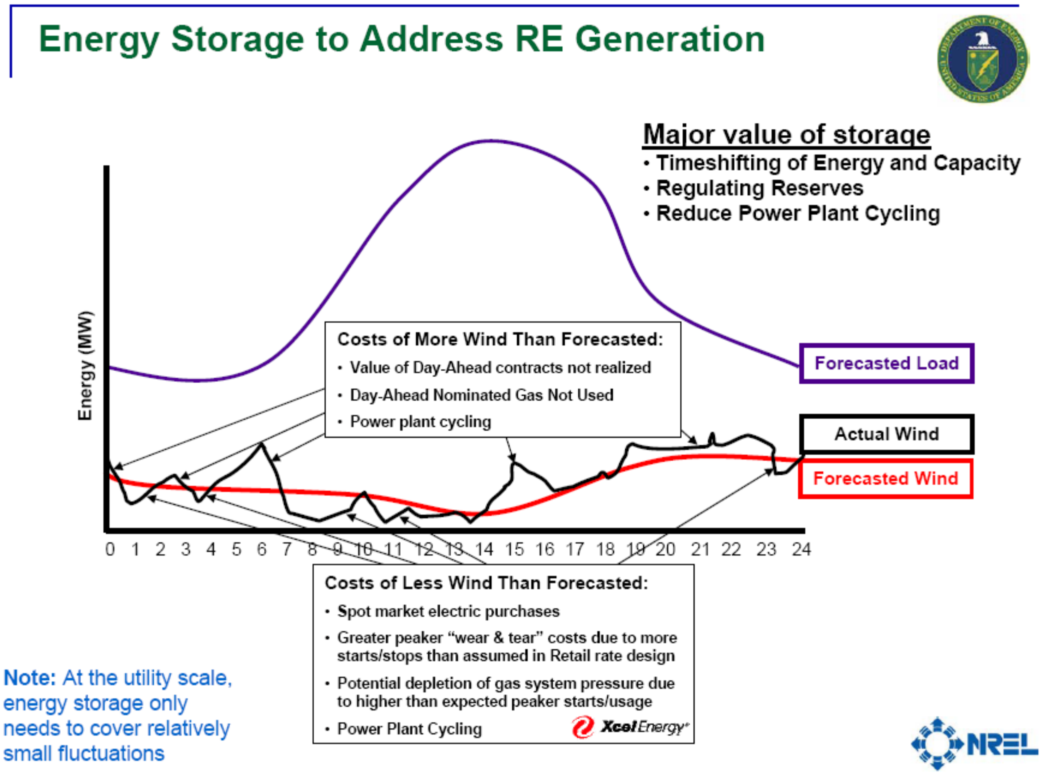
4. Easier integration of renewable sources of energy, such as wind and solar, thus allowing a higher penetration of renewables;

5. More efficient delivery of services needed for grid operation;

6. Increased asset utilization of existing power generation and delivery infrastructure;

7. Deferral of asset acquisition or upgrading; and

8. Improved reliability, power quality, and security of the grid.



Energy Storage to Address RE Generation

Major value of storage
- Timeshifting of Energy and Capacity
- Regulating Reserves
- Reduce Power Plant Cycling

Costs of More Wind Than Forecasted:
- Value of Day-Ahead contracts not realized
- Day-Ahead Nominated Gas Not Used
- Power plant cycling

Costs of Less Wind Than Forecasted:
- Spot market electric purchases
- Greater peaker “wear & tear” costs due to more starts/stops than assumed in Retail rate design
- Potential depletion of gas system pressure due to higher than expected peaker starts/usage
- Power Plant Cycling

Note: At the utility scale, energy storage only needs to cover relatively small fluctuations

Figure 6-1 Example of impact of wind intermittency on the 24-hour daily cycle of power generation and use. Source: National Renewable Energy Laboratory.

Status of Present and Ultimate Industrial Technology Development

In the transportation area, energy storage is already being used in HEVs. The current nickel-metal-hydride (NiMH) battery technology will soon be eclipsed by lithium-ion (Li-ion) batteries, which offer higher energy and power density. In HEVs, batteries and related systems are often oversized in order to meet performance goals at low temperature. Improvement of low-temperature performance would result in a practical increase in energy density, due to the opportunity to “right size” the batteries or related components. PHEVs and EVs are starting to become commercially available, although the present high cost of such batteries and vehicles will likely limit widespread adoption.

In the utility industry, energy storage for the grid is just starting to be deployed more widely. Traditionally, electricity energy storage systems have not been produced at the scale required for use in the grid. This, however, is changing, and several companies are pursuing utility-scale energy storage now. Demonstration projects using various technologies have shown the potential of flow batteries, flywheels, and other battery technologies. In November 2009, the U.S. Department of Energy announced the award of $620 million for smart grid demonstrations and energy storage projects. This is expected to further accelerate development and deployment of grid-scale energy storage.

The barriers to wider penetration of energy storage in transportation and grid applications are cost, life (durability), safety, and efficiency. The two biggest cost drivers in an electrochemical storage system are the materials costs and the processing/production costs. The current cost must be reduced by factors of two to five to achieve the widespread deployment that is needed to truly address the nation's challenges in both the transportation and utility sectors.

Context and Background for the Priority Research Directions (PRDs)

The key industrial targets for electric energy storage for transportation are dollars per watt-hour ($/Wh), expanded temperature range, life of 20 years, and 2x energy density. Stationary grid applications share the cost and lifetime targets, but high energy density is less important than high efficiency. Although the breakthrough technology is not yet known, it is clear that the energy storage field would benefit from higher energy density (watt-hours per kilogram [Wh/kg] and watt-hours per liter [Wh/l]) at lower cost ($/Wh), while extending life during usage. This means that the energy storage technology should have improved cycle life and calendar life (durability over time), while operating in a wider temperature range.

The options for storing energy for large-scale applications, such as transportation and the grid, are currently (1) batteries and supercapacitors, (2) fuel cells, (3) flow batteries, (4) flywheels, and (5) compressed gas and pumped hydro. Each of these existing energy storage technologies has its own limitations, which are detailed below.

1. Batteries and supercapacitors have low energy density and high cost compared to gasoline and diesel, when used for transportation. Advanced lead batteries have a cost structure needed for large-grid storage, but have issues with lifetime, maintenance, and operating temperature range. For Li-ion batteries, industry experts predict 5% to 10% cost reductions per year, with a floor near $300 per kilowatt-hour under best-case scenarios for systems that have the long life required for transportation and grid applications. As with all batteries, the floor for cost exists because every battery cell has expensive components such as the separator, active material, current collector foil, and packaging. Only the active material stores energy; everything else is "overhead" or dead weight that is necessary to make the battery function. A better energy storage system would maximize the active material, but reduce the overhead, which in turn would reduce cost ($/Wh). Hence, the near-term industry approach is to move to thicker electrodes and larger-sized cells (>40 ampere-hours [Ah]) that reduce packaging, but still have all of the other inert materials, such as separator and foil.

2. Fuel cells do not, strictly speaking, constitute electricity energy storage, but compete with batteries, supercapacitors, and flywheels in some applications. They have the advantage of using hydrogen, a fuel that can be quickly pumped into the vehicle, allowing for fast charge. But they are very costly and pose challenges for storing hydrogen onboard the vehicle, in addition to the infrastructure challenge of an adequately supportive hydrogen economy.
3. Flow batteries have even lower energy density than conventional batteries — too low for transportation applications, but they are easily scalable to large systems.
4. Flywheels are being developed for grid applications, but they are presently too costly and plagued with concerns about product life. Efforts are underway to increase size and storage capacity, and to increase life and product reliability.
5. Finally, compressed gas and pumped hydro are well-known solutions that can be applied in certain situations.

While there is little opportunity for research to open up major new avenues of improvement in compressed gas and pumped hydro, the other technologies — particularly batteries and capacitors — offer major research opportunities.

The ideal energy storage system for transportation could provide a viable alternative to burning liquid hydrocarbon fuels, but would avoid the critical drawbacks with respect to the environment, sustainability, and energy security. For electric vehicles, such a storage system requires significantly increased energy density compared to current batteries. It would store the energy using a material that need not be compressed or liquefied cryogenically, which are energy-intensive processes. It should be easy to scale up to store many tens or hundreds of kilowatt-hours (kWh). New architectures might be developed that leverage existing technologies to dramatically increase energy density while reducing cost. Alternatively, completely new materials and approaches to store energy might have to be developed to achieve desired metrics.

Brief Description of Energy Storage PRDs

In this report, we focus on research for electrochemical storage devices, such as batteries and capacitors, for either transportation or grid applications. These are complex systems in which electrical, chemical, and mechanical processes take place concurrently to achieve storage functionality. Past research has focused on improving basic performance characteristics such as energy density, power density, and life. Recent successes in these areas have led to technologies providing a first significant step in meeting performance requirements for electrification of transportation and grid integration of renewables. Now, the most impactful research will result in improved economics of such systems as expressed via \$/Wh or dollars per watt (\$/W). As electrochemical storage devices have an intrinsically multidisciplinary character, so too do the primary research directions identified at the Basic Energy Sciences Advisory Committee (BESAC) Workshop. These are (1) new materials, (2) novel structures and processes, and (3) interface understanding and control, as indicated in Fig. 6-2, each occurring within a context of systems understanding.

A critical element underlying these research directions is the need for systems-level understanding. Much earlier basic research has focused on an isolated element of the electrochemical system rather than on how the element would function in a full system that includes other necessary system components. Thus, while the PRDs set out specific missions, they should all be pursued in a systems context. Similarly, while the PRDs address key metrics, improvement of one metric may impact others, because they are interrelated in an interactive system. For example, improvements in low-temperature performance, stable interfaces, architectures, and processing potentially affect both practical energy density and cost.

New analytical tools are also needed in the context of the PRD's exploration efforts, particularly for interrogating interfaces.

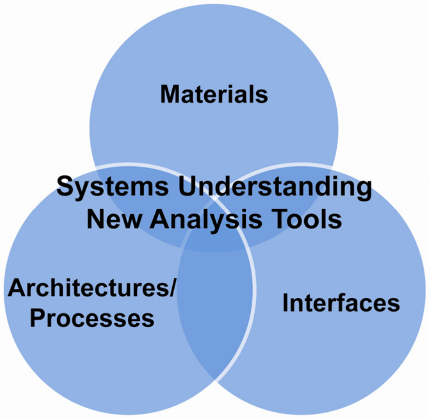


Figure 6-2 Relationship of energy storage PRDs.

Figure 6-2 shows a conceptual view of the relationship between three PRDs, which are further described here. (1) New materials are needed to fundamentally increase the energy density, specific energy, and power of electrochemical systems. New materials include not only the active materials, anode, and cathode, but also electrolyte systems that critically impact temperature performance of the system. (2) New architectures are sought to increase performance (energy and power density) while reducing the cost. This might be achieved by materials with higher energy density or systems that minimize the inert materials that do not contribute directly to energy storage. New processes linked with architecture will be needed. (3) The understanding and control of interfaces presents a significant challenge. Electrochemistry is a surface phenomenon, yet often, the interfaces are not understood or controlled, and they change significantly over time, affecting the power capacity of a system. Thus, in-depth understanding of interfaces — how to control and stabilize them over time — is still needed. These research directions overlap considerably with those developed in an earlier Basic Research Needs Report on Electric Energy Storage [2].

III. PRIORITY RESEARCH DIRECTIONS

A. PRD #1. New Materials for Enhanced Battery Performance

1. Problem Statement

Although advanced lead batteries have the cost structure needed for large-grid storage, they have issues with lifetime, maintenance, and operating temperature range. Advanced Li-ion batteries are approaching broad application in electric vehicles, but still do not meet desired cost and lifetime requirements, and also have a limited operating temperature range. Metal-ion batteries have the potential for very low cost but have severe challenges with life and reliability, with solutions expected to take ten years or more. In sum, significant challenges face energy storage technologies in cost, energy density, lifetime, and operating temperature range, and new materials are needed to make significant breakthroughs.

2. Executive Summary

New materials, including new cathode, anode, and electrolyte materials, are essential to meeting industry needs for breakthroughs to significantly reduce \$/Wh, and increase Wh/kg and life. One scientific challenge is recognizing the system-level linkages in which many performance characteristics must be simultaneously achieved. The research directions include chemical doping to engineer band gaps, coating particles with conductive material to improve electrical conductivity, reducing cost by direct formation of electrode materials from precursors, and developing carbon monoxide (Co)-free cathode materials and new nanocomposites with flexible graphitic backbones. The ultimate impact is lower cost, more functional electrical energy storage systems expanding existing consumer applications, and enabling larger-scale systems for transportation, industrial, commercial, and grid applications.

3. Context and Background for PRD #1

An electrochemical storage device consists of two electrodes separated by an ionically conductive but electrically insulating separator, with an electrolyte contained within a suitable package. Currently, materials constitute the most significant cost in most electrochemical storage devices. New cathode, anode, and electrolyte materials hold the keys to improved performance and could significantly open the market.

4. Industry Need

The most significant challenge facing batteries for transportation is the improvement of the economic price/performance metric, or stated another way, \$/Wh at the materials level. Research in improving energy density coupled with an economic measure, would produce the greatest impact. At the same time, weight needs to be reduced, temperature range for operation increased, and lifetime extended. The desired levels of improvement are as follows:

- \$/Wh needs to improve two to five times over current levels;
- Wh/kg, Wh/l need to improve two times;
- Temperature range needs to improve from −10° to 60°Celsius (C) to −30° to 85°C, ideally up to 120°C; and
- Life needs to improve to 10 to 20 years.

For grid-storage applications. the significant challenges include cost and performance, but also capacity in the 100 megawatt-hour (MWh) range, and efficiency. Temperature range is less critical, as stationary grid storage can be housed in a controlled environment.

5. Scientific Challenges

Historically, new materials development has often focused on a single material such as anode, cathode, or electrolyte, which does not guarantee improvement in overall battery performance. A battery is a system, and the integrated functionality of all components must be addressed.

The most significant challenge in discovering new active materials is lack of a fundamental framework to predict a sufficiently complete set of properties to achieve all performance and economic requirements. Currently, combinations of ab initio or mechanistic models can predict properties such as electrochemical potential, capacity, and certain conductivity and mass transfer characteristics, but such performance characteristics as irreversible capacity loss, abuse tolerance, and most significantly, lifetime, are beyond current theoretical frameworks. Development of theoretical frameworks that more comprehensively cover material property prediction and integrate the effects of a variety of materials, for example, cathode or anode activity with electrolyte, would improve the modeling.

Lithium-ion batteries are likely to be a dominant technology for the foreseeable future. Achieving higher energy density, lower cost, and longer lifetime while maintaining safety requires (1) new cathodes that easily accept lithium ions as intercalants or as substitutions with stable structures and little lattice constant change over wide lithium concentrations; (2) non-flammable electrolytes with higher ionic conductivity and low reactance with the electrodes; and (3) anodes with improved solid-electrolyte interface layers.

Sodium batteries offer advantages of high energy and power density and high efficiency for heavy-duty transportation such as locomotives or forklifts and for utility-scale grid storage. The major challenges are safety and corrosion arising from the high operating temperatures (above 300°C) that are needed to promote electrolyte ionic conductivity. Finding low-temperature electrolytes with high-sodium ionic conductivity is a major challenge. Sodium anodes can operate with a variety of cathodes, including sulfur and transition metal halides such as nickel/nickel chloride. Identifying cathode materials compatible with low-temperature electrolytes requires significant research.

6. Research Directions

- A number of candidates for Li-ion battery electrolytes are less expansive, are more stable, have higher capacity, and exhibit less volume expansion on discharging than the lithium cobalt spinel ($LiCoO_2$) now in common use. The challenge is to select materials classes with desirable properties and optimize them by adjusting composition. Lithium nickel oxide ($LiNiO_2$) is lower in cost and higher in energy density than $LiCoO_2$, but less stable. Layered alloys of $Li(Ni_xCo_{1-x})O_2$ can be used to tune cathode properties. Adding manganese (Mn) allows the structure and the site exchange disorder of cobalt (Co), nickel (Ni), and Mn on the lithium (Li) site to be controlled. Lithium manganese spinel ($LiMn_2O_4$) has three-dimensional lithiation pathways in contrast to the planar pathways of $LiCoO_2$, and has lower cost but lower energy density; its properties can be tuned by alloying with Ni, Co, and iron (Fe). Phosphates such as lithium iron phosphate ($LiFePO_4$) are promising cathode materials (see Fig. 6-3), where iron phosphide (Fe_2P) can be added to increase electronic conductivity. Other phosphates such as lithium manganese phosphate ($LiMnPO_4$) and lithium cobalt phosphate ($LiCoPO_4$) are promising, and mixed compositions with Fe, Co, and Mn content provide a rich phase space to be explored [3].

- Although graphite is an effective anode for Li-ion batteries, its operation depends on formation of a complex solid-electrolyte interface layer between anode and electrolyte that prevents decomposition of the electrolyte by the anode, yet permits transport of lithium ions. Other anodes that have higher energy density or do not require a solid-electrolyte interface layer are possible. Promising candidates include silicon [4], carbon nanotubes [5], $LiTi_{15}O_5$ [6], $LiTi_2O_4$ [7], cupric oxide (CuO) [8], titanium dioxide (TiO_2) [9], tin dioxide (SnO_2) [10], and grapheme [11]. Nanostructuring plays a key role in many of these anode materials, to facilitate lithiation and mitigate large volume changes.

- The electrolyte in battery or electrochemical capacitor systems drives and restricts many of the operating characteristics as well as the range of compatible materials that can be used for cathodes and anodes. Ideal electrolytes have a wide bandgaps allowing high-voltage operation, high ionic conductivity allowing fast charge and discharge, low cost, and high stability [12,13]. The number of possible electrolytes is large; a few have been selected for development based on experience and empiricism, leaving many more to be explored. The lithium hexafluorophosphate ($LiPF_6$) electrolyte in Li-ion batteries can produce hydrogen fluoride that dissolves cathodes, triggering migration of cathode constituents to anodes and producing capacity loss. New electrolytes include boron salts for their higher stability, provided suitable solid-electrolyte interfaces can be developed. Lithium bis(oxalate)borate ($LiB(C_2O_4)_2$) (LiBOB) is interesting for its potential low cost, ready availability, and good ionic conductivity. With suitable modification, lithium borohydride ($LiBH_4$) offers high ionic conductivity at room temperature [14]. Polymer electrolytes are gaining popularity for their potentially high energy densities, close to the limit for Li-ion batteries. Ionic liquids, with high ion mobility at low temperature, low vapor pressure, and non-flammability offer interesting possibilities [11,12,15].

- The high operating temperature of sodium batteries (above 300°C) imposes many restrictions on the materials that can be used and requires special attention to safety with regard to the explosive reaction of sodium with water. Lower operating temperatures require tuning the properties of the standard electrolyte beta-alumina (Al_2O_3) with additives to get adequate ionic conductivity. New polymer-based electrolytes such as polyvinylidene fluoride–hexafluoropropene (PVdF) [16] and polyethylene oxide [17] — allow operation as low as 25° to 90°C. At low temperature, sodium and sulfur remain promising candidates for anode and cathode materials, with transition metal halides such as nickel chloride and ferrous chloride receiving strong attention as alternative cathodes [18].

- Development of materials that can dramatically reduce processing cost is also important. Current electrode production methods involve sequential formulating, mixing, coating, and pressing electrode constituent components. Approaches that probe direct formation of electrode from precursor active material components offers dramatic potential for improved $/Wh.

- Development of materials with multiple functions could bring major benefits. Currently, both binders and conductive additives are used in many electrode formulations for energy storage devices. Development of intrinsically conductive binders or of functionalized active materials could obviate the non-active constituents within the cell.

7. Potential Impact

Improvements in the combination of anode, cathode, and electrolyte materials will provide lower-cost energy storage systems, further expanding consumer market applications and enabling large-scale or distributed energy storage systems for transportation, industrial, commercial, and grid utility applications.

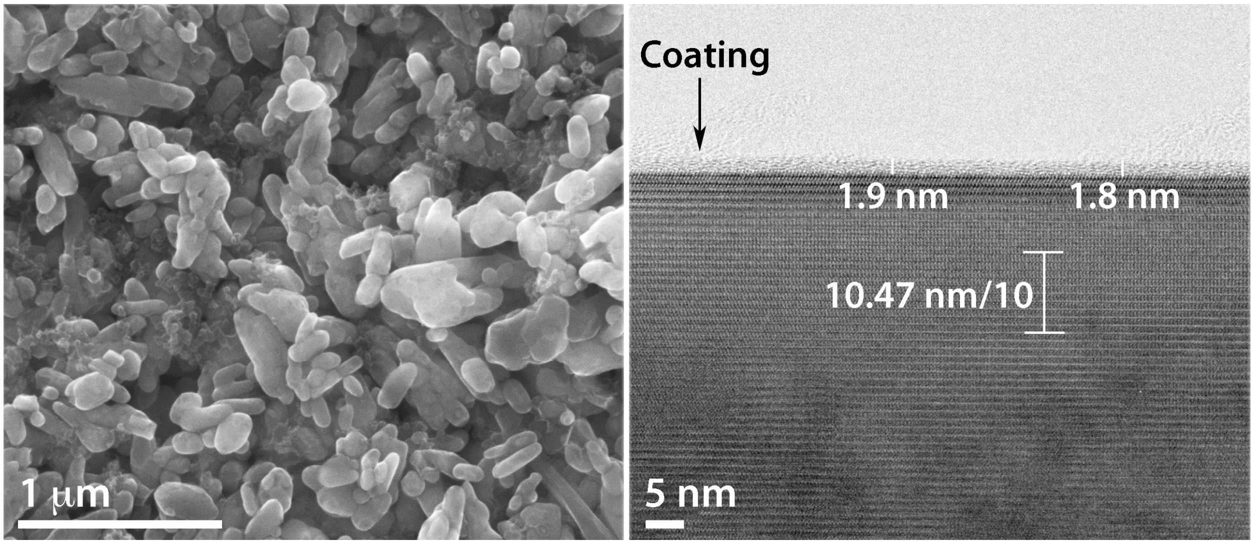


Figure 6-3 A scanning electron microscope (SEM) image (left) of a pristine $LiFePO_4$ cathode showing good particle size distribution and lack of excessive agglomeration. The high-resolution transmission electron microscope (TEM) image (right) of an individual $LiFePO_4$ cathode particle shows the crystalline nature of the particle. Also, a thin carbon coating on the particle surface, which is present to enhance electrical conductivity, is visible. Source: U. Sharma and H. Shen, Evans Analytical Group.

B. PRD #2. New Architectures for Electric Energy Storage

1. Problem Statement

Innovation in the spatial relationship between device constituent materials, architecture, and processes for creation of new architecture represent key opportunities to improve the performance and cost of energy storage devices. From the microscopic to the macroscopic, architecture determines the performance capabilities of the energy storage device.

2. Executive Summary

To maximize performance and value, batteries are designed to optimize the ratio of active materials (cathode and anode) to inactive materials (separator, electrolyte, current collector, packaging, and electrode additives such as binders or conductive additives), subject to limitations posed by (1) the intrinsic capabilities of charge/mass transfer of the various materials and (2) practical constraints associated with device fabrication. The industry need is to achieve significant advances in cost and performance. A scientific challenge is to innovate microscopic configurations such as the separator with an electrode, and new processes beyond conventional slurry coating. Research directions include morphology modifications and improved microscopic models. The potential impact is to enable broad use of electrochemical storage in transportation and grid applications.

3. Context and Background for PRD #2

The importance of energy storage has grown over the past decades and has reached an unprecedented level as our nation electrifies transportation and integrates alternative energy, especially intermittent wind and solar energy, into our electrical utility grid, and as consumers' use of portable wireless electronic devices increases. Reduction of carbon emissions and the consequential reduction in global warming is now an international imperative, with nations around the world striving for leadership. While tremendous effort has already addressed the need to achieve electrochemical storage in batteries and supercapacitors with lower cost and higher performance, a deeper scientific understanding of the processes involved and innovation in the architecture and process would open up further progress and assure broad impact in storage for electric vehicle transportation and utility-scale applications.

4. Industry Need

The most significant challenge facing the field is improving the economic price/performance metric, or stated another way, $/Wh. At the same time, weight needs to be reduced, temperature range for operation increased, and lifetime extended.

5. Scientific Challenge

When considering the "architecture" of electrochemical energy storage, one normally focuses on the overall device structure at the macroscopic level. However, the scientific challenge associated with cost and performance lies in architecture at a microscopic and even atomic scale. An example is the interface between a dielectric separator and the active electrodes of an energy storage device, where separator function might be configured with the active electrode as an integrated multifunctional component intimately tied to the electrode itself. The scientific challenge is to create and control a chemical and physical process that will lead ultimately to a manufacturing process for the interface.

The importance of architecture for batteries is illustrated in Fig. 6-4, showing the energy level diagram of the anode, electrolyte, cathode, and solid-electrolyte interfaces [12]. The architecture of the battery must integrate these four elements so that they work together synergistically; if any one of them is out of step, system functionality and performance are lost.

Improved architectures that integrate multiple components would produce several benefits. Consider that an electrode has to be slurry-coated at high cost for manufacturing, capital equipment, facilities, and utilities. The conventional process is not “green”; it consumes a great deal of energy and is deleterious to pure electrode performance. Finding a way to assemble electrodes using alternate strategies such as building them from the ground up using chemical vapor deposition or other techniques would be attractive, but requires scientific understanding of the growth process and component interactions. Active materials are already created this way for energy storage, but have yet to approach cost and performance targets to meet industry needs. Finding a new way to create active electrode structures from an integrated perspective, where discreet components brought together in seamless unity, should be the baseline.

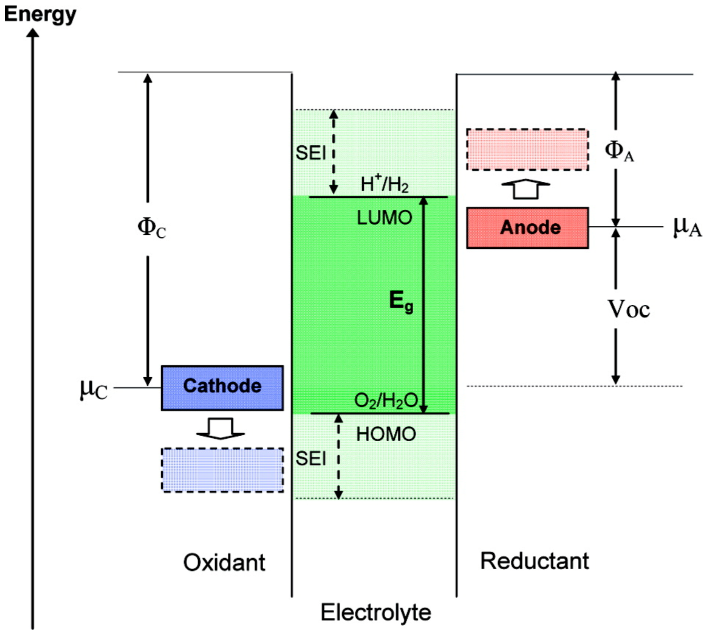


Figure 6-4 The electrochemically active anode and cathode must fit energetically with the electrochemically passive electrolyte and solid-electrolyte interfaces (SEI), to form a functionally operational architecture. The Fermi level of the anode and cathode are μ_A and μ_C, respectively; Φ_A and Φ_B are their workfunctions; V_{OC} is the open circuit voltage between anode and cathode; E_g is the electronic energy gap in the electrolyte; and SEI is the solid-electrolyte interface that passivates the reaction between anode or cathode and electrolyte. Source: After [13].

6. Research Directions

1. *Combining active materials at the microscopic level for new performance and cost advantages*. Examples would be to find new ways to integrate active lithium into carbon matrices to improve energy density and reduce cost. Some methods exist today; further directions include integrated separator/electrode interfaces by "assembling" the separator to the electrode, resulting in a single component with multifunctional performance.

2. *Understanding the electrolyte and its interfaces with the energy storage active materials, and then devising electrolyte solutions that provide more efficient integrated function.* In the case of ultracapacitors this would mean increasing the surface area of the electrodes that is accessed by the electrolyte and more intimate contact between the two. This could include morphology modifications to the active materials such that they interact with the electrolytes in novel ways. This could add the energy density necessary to reduce cost.

3. *Attention to anode and cathode interactions and the ability to build low-cost electrodes by addressing the drawbacks of the current slurry coating processes.* Research robust, energy-dense electrodes without slurry coating by focusing on fixing active materials to conductive backplanes, as well as getting the particles to bind together in other ways. The binding is a key to creating high-performance electrodes.

4. *Development of predictive 3-D microstructurally resolved performance and degradation models and accurate accelerated life methodologies,* which will expedite lifetime validation.

7. Potential Impact

Reductions in energy density and cost enabled by innovations in microscopic architecture could have broad impact in expanding today's electric storage applications and providing novel energy solutions for tomorrow.

C. PRD #3. Panel 4: Understanding and Controlling Heterogeneous Interfaces

1. Problem Statement

Interfaces are critical to the performance and functionality of energy storage systems. There is an urgent need for breakthroughs in high-performing interfaces in batteries and supercapacitors to achieve the performance and cost targets needed for transportation via plug-in electric vehicles and in utility-scale storage to address and mitigate the intermittency of renewable energy sources like wind and solar.

2. Executive Summary

In order to better design and control interfaces between electrolytes and cathodes or anodes, atomic-level understanding of their in situ structure, composition, and dynamics is essential. Theoretical and experimental tools need to be developed to address this need. During manufacture and use, the most complex interfaces in batteries and supercapacitors are exposed to reactive chemical environments including air, intentional additives, and impurities. The interface is often a complex, chemically inhomogeneous layer many nanometers thick that may be amorphous. The properties of these interfacial layers often determine the performance and durability of the system. Our understanding of these layers is rudimentary and empirical; systematic investigations and deeper understanding are needed.

3. Context and Background for PRD #3

The interfaces between electrolyte and cathode or anode are key enablers and limitations to battery performance, especially rates of charge/discharge, shelf life, and durability in use. In particular, all battery and supercapacitor systems depend on interfaces to bind or transfer ions and promote stability.

4. Industry Need

The broad industry need is for batteries and supercapacitors with lower cost and higher energy density, along with longer lifetime and higher-temperature performance. As part of meeting this challenge, a focus on understanding and improving interfaces is critical. Novel materials systems for anodes and cathodes in lithium batteries are the subject of current research interest to increase energy density, with a goal of a factor of two to five. A factor of 10 is the “holy grail” for batteries — an absolute limit imposed by the properties of the chemical elements in the periodic table. At the same time, decreasing materials cost is imperative.

5. Scientific Challenges

Lithium batteries are among the most advanced and complex energy storage systems, in that cations must pass through an inhomogeneous interface between a solid anode or cathode and an electrolyte, and then intercalate into a solid. It is well known that a reaction layer forms on the surface of both electrodes, and that this reaction layer prevents rapid decomposition of the electrolyte and the active electrode materials. There is high potential to manipulate this layer to affect the cyclability and life of the battery, but greater understanding of ion transport through the interface and the interface contribution to the kinetic stability of the system is needed. Further, the chemical and physical behavior of these layers can be strongly temperature-dependent.

Supercapacitors are somewhat simpler than lithium batteries, but require deeper understanding to improve energy density or increase their voltage limits. Supercapacitor performance is dependent simply on surface area of the electrode materials (usually particular forms of carbon black), but also on the size and distribution of pore sizes. Advanced theoretical and experimental tools need to be applied to the nature of the electrolyte/carbon nanoporous surfaces. There is a strong driver to increase the energy density by increasing the maximum voltage that can be sustained over hundreds of thousands of cycles, since the energy density is proportional to the voltage squared. As in lithium batteries, durability decreases rapidly with increasing temperature.

Tool development to characterize battery interfaces, including electrodes/electrolyte and current collector/active material, needs to be accelerated. There are wide opportunities at the national laboratory user facilities to develop tools such as imaging, structure, and spectroscopy, using electrons, X-rays, and neutrons for the study of battery and electrochemical capacitor interfaces. New microscopic probes will accelerate the research to improve the energy, power, cost, life, and cost attributes of energy storage systems. In situ studies of chemical and microstructure evolution, for instance, using synchrotron radiation penetrating active battery housings, are a powerful tool, as illustrated by recent work on metal halide batteries in Fig. 6-5.

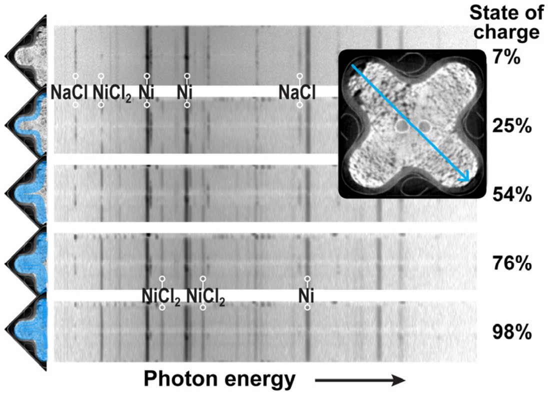


Figure 6-5 Cross-sectional X-ray diffraction patterns of General Electric's (GE's) sodium metal halide battery taken at various times during charging of the $Na/MCl_2 \Leftrightarrow NaCl/M$ battery, taken at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. Each strip on the right represents a position along the vertical line on the left; the dark lines within each strip indicate which phases are present at that location and thus, reveal changes in battery chemistry. Source: J. Rujssenbeek and Y. Gao, GE Global Research.

6. Research Directions

Graphite anodes in Li-ion batteries require solid-electrolyte interfaces to prevent decomposition of the anode by the $LiPF_6$ electrolyte, to prevent solvated lithium ions from intercalating into and exfoliating the graphite, and to promote Li-ion exchange between anode and electrolyte [19]. Mild oxidation removes active sites from the graphite edges, reduces decomposition of the electrolyte on the first charging cycle, and creates a dense layer of oxides revealed by infrared spectra to become part of the solid-electrolyte interface. Oxidation produces nanochannels and micropores that promote reversible lithium storage. Metals such as nickel, zinc, silver, and aluminum can be deposited on the graphite anode to improve the reversible capacity, kinetics, and cycling behavior. Polymer coatings can improve electrochemical performance for Coulombic efficiency in the first cycle, reversible capacity, and kinetics.

Each of the cathodes proposed for Li-ion batteries requires its special coatings to enhance performance [18]. $LiCoO_2$ is often coated with magnesium oxide (MgO), SnO_2, Al_2O_3, or zirconium dioxide (ZrO_2) to prevent phase transitions of the cathode that degrade reversible lithiation. $LiMn_2O_4$ can be used to improve thermal and chemical stability. $LiNiO_2$ can be coated with ZrO_2, lithium diborate ($Li_2O{\cdot}2B_2O_3$) glass, MgO, and TiO_2 to retard decomposition and maintain capacity with cycling. $LiMn_2O_4$ improves its capacity-fading, Mn dissolution at high temperature and high-rate capability when coated with $Li_2O{\cdot}2B_2O_3$ glass, MgO, Al_2O_3, lithium aluminum oxide ($LiAlO_2$), potassium manganese trifluoride ($KMnF_3$), lithium cobalt oxide ($Li_{1-x}CoO_2$), $LiCo_xMn_{2-x}O_4$, silicon dioxide (SiO_2), carbon, and polymers. Aluminum fluoride (AlF_3) is an effective coating of $LiFePO_4$ cathodes for preventing dissolution of Fe in the $LiPF_6$ electrolyte and for lowering the charge transfer resistance [20].

Most investigations of solid-electrolyte interfaces for the functionality of batteries and electrochemical capacitors are empirical and not systematic, often examining the impact of a single coating on a single property, instead of interactions among multiple coatings and outcomes. The enormous number of compositions, structures, and morphologies of coatings can be addressed effectively only with advanced tools like simulation based on density functional theory [21,22,23], in situ experiments using X-rays [24], electrons [25], and neutrons [26], scanning probe microscopy [19], and systematic variation of compositions. Advanced techniques such as atomic layer deposition are promising synthesis tools for precise synthesis of interface structures [27].

7. Potential Impact

Improved interface performance in electrochemical storage is key to enhanced battery performance and reduced cost per kWh. Significant progress will unlock major markets in the transportation and utility-storage sectors.

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Chapter 7: Panel 5 — Electric Power Grid Technologies
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I. EXECUTIVE SUMMARY

The electric power grid is a major engineering achievement of the 20th century. Given the inexorable growth in demand for electricity, its versatility in providing energy services, the opportunities for electrification of transportation and the need for transmission of abundant renewable power resources to distant load centers, electricity is one of the fundamental enabling clean energy technologies of the 21st century. In meeting the growing need for electricity, the grid faces huge challenges, many of which require fundamental scientific understanding and breakthroughs in basic materials and in system-level integration. The Priority Research Directions for the electricity grid include: (1) higher performance power electronic materials; (2) superconductor materials for underground transmission and for increased power density and performance in generators, motors, and fault current limiters; (3) electrically insulating materials with improved dielectric and thermal properties; and (4) novel composite electrical conductors for high-temperature, low-sag overhead transmission lines. System-level scientific challenges include credible modeling and simulation tools, and measurement, monitoring, and control of the high-dimensional complex interactive electric grid system covering system dynamics with time scales from milliseconds to days. The potential impact of success in these research directions will be a higher transmission capacity and more efficient, stable, and reliable grid, capable of meeting the clean energy demands of this century.

Role of Electric Power Grid Technologies in National Energy Picture

The electric power grid is a major engineering achievement of the 20th century and is one of the fundamental enabling clean energy technologies of the 21st century. Electricity has the unique ability to convey both energy and information, delivering energy to the user with no emissions at the point of use, and providing an increasing array of innovative products, services, and applications in factories, offices, homes, campuses, complexes, and communities. It is fundamental to our civilization.

In 1940, 10% of U.S. primary energy was converted to electricity; as shown in Fig. 7-1, by 1970 that percentage had grown to 25%, and today it is roughly 40%. If the current vision of electrifying transportation to reduce dependence on petroleum becomes a reality, as much as 60% of all primary energy may be in the form of electricity by 2050. This expansion of electricity use has come on top of overall growth in demand for power, leading to extraordinary demands on the power grid that supplies it.

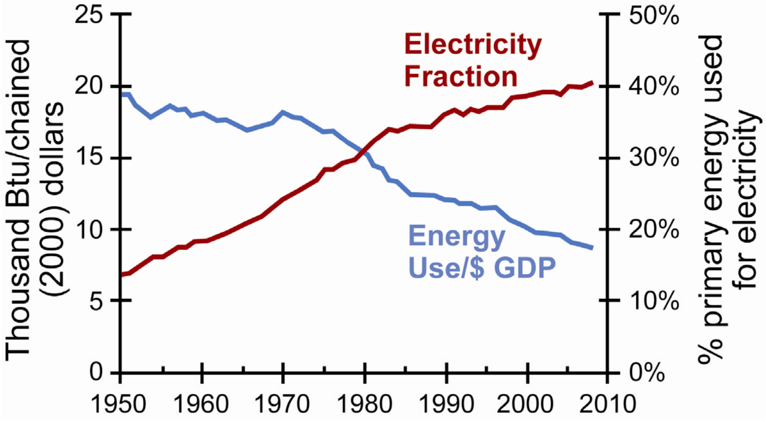

Figure 7-1 Electricity use is increasing in both absolute and relative terms. And it is taking less and less energy per $/GDP to fuel the economy. Source: Figure 13.3 in [1], and information in [2].

The electricity delivery system — the *grid* — is a fundamental infrastructure of modern society, yet the current North American grid is a patchwork of legacy designs that evolved over a century, and it is pressed today into duties not anticipated by its designers. The grid is, in fact, a system of systems. These systems include three physical network systems: (1) the fuel and energy resource network, (2) the power flow network, and (3) a communications and controls network. Overlaying these physical networks and creating additional constraints on the physical networks are (4) a money exchange network, (5) a business network, and (6) a government and regulatory network. The essential physical network — the power system of generation, transmission, distribution, and end user or customer — is linked together by the interplay of the linkages within and between the various financial, business, and regulatory networks. All the elements of the grid — generating facilities, the delivery system consisting of the transmission and distribution systems (underground cables, overhead power lines, transformers, and switchgear, plus capacitors and inductors) and the end uses — are interconnected, and the entire system is in fact one extremely complex machine. At the core of this machine is the power flow from generator to end use across the grid, which in the United States includes hundreds of thousands of miles of transmission lines and millions of miles of distribution. It is not only a system of high dimension, but a complex, non-linear system that today lacks a comprehensive fundamental theory that can predict behavior under all relevant conditions and timescales.

The electric power grid will play a critically important role in the clean energy technology of the future. One aspect of this is the needed improvements in grid efficiency to reduce the 8% of approximately one terawatt of U.S. electricity consumption that is presently lost in resistance between the generator and the customer meter. But even more important than this efficiency improvement is the need for expansion of capacity to meet the energy demands of our growing economy, and particularly, of electrifying transportation with plug-in vehicles. The challenge of expansion is most extreme in urban areas, where high-power overhead transmission lines are no longer aesthetically acceptable, and the underground infrastructure of gas pipes, communications cables, water mains, and power cables is so dense that there is literally no room to install conventional underground cables, since these require significant spacing from other infrastructure because of the heat and electromagnetic fields they emit.

The growing grids in urban areas also bring another critical problem, which more and more utilities are facing: as additional generation is added, the potential fault-duty currents that arise because of short circuits increase proportionately. Some grids are already reaching levels at the rated capacity limits of switchgear. These limits cannot be exceeded without risk of destroying the generation and delivery infrastructure of the grid. With increasing capacity and complexity, other stability issues leading to brownouts and blackouts are also increasing. In the present grid, electricity flows passively, following the paths of least impedance, as determined by Kirchoff's laws, sometimes in destructive patterns like those that led to the extensive power blackout in the northeastern United States in 2003. New methods of actively controlling current flow and dealing with fault currents and other grid instabilities are urgently needed.

The economic significance of electricity is staggering. It is one of the largest and most capital-intensive sectors of the economy. Total asset value is estimated to exceed $800 billion, with approximately 60% invested in power plants, 30% in distribution facilities, and 10% in transmission facilities. Annual electric revenues – the Nation's "electric bill" – are about $247 billion, paid by America's 131 million electricity customers, which includes nearly every business and household.

"GRID 2030" A NATIONAL VISION FOR ELECTRICITY'S SECOND 100 YEARS

Another critical clean energy challenge is integrating renewable electricity resources into the grid. This is essential to achieving at least two goals announced by President Obama in early 2009: (1) reducing greenhouse gas emissions by 83% from 2005 levels by 2050* and (2) significantly reducing petroleum consumption and imports. Grid advancements play an important role in greenhouse gas mitigation by facilitating the deployment of low-carbon power generation technologies and by enabling optimal operation of the grid. While petroleum accounts for only about 3% of total U.S. electric generation [3], the electrification of the vehicle fleet using non-petroleum sources can enable a major reduction in petroleum consumption and carbon intensity over time.

A central challenge to deploying today's best and most cost-effective renewable technologies is linking areas of high renewable resources (which are often located in sparsely populated areas) to regions of high population density, where load is highest. This is especially true for wind and solar thermal electric power. For example, the Eastern Wind Integration Study and the Western Wind and Solar Integration Study both found that a two-pronged development scenario — developing the best local renewable resources, combined with building transmission to deliver electricity from regions where these resources are most plentiful — provided the most cost savings and best reliability when meeting a 20% to 35% renewable energy goal [4,5]. However, expansion of renewable energy and other low-carbon technologies will likely be limited by the antiquated grid infrastructure, unless key technical and institutional barriers that slow down new transmission construction can be overcome. These studies also show that significant changes in how the grid is operated will be needed to address the increased complexity, variability, and uncertainty of incorporating high levels of renewable resources.

Status of Present and Ultimate Industrial Technology Deployment

The current grid was not holistically designed and developed, but rather, evolved over time in response to local needs and opportunities to cooperate regionally to share resources and reduce risks. Still, it is a remarkable engineering achievement, and operates today with about 92% efficiency from generation station output to customer meter. Today there are 30,000 transmission paths; over 180,000 miles of high-voltage transmission lines; 14,000 transmission substations; and some 11 million miles of distribution lines that connect to customers. The electric power industry is a fragmented industry without a common voice, comprising over 3170 traditional electric utilities: 239 are investor-owned, 2009 utilities are publicly owned, 912 are consumer owned rural cooperatives, and 10 are federal electric utilities.

The future grid should be a smart grid, a fully automated power delivery network ensuring a two-way flow of electricity and information between a few thousand conventional generators and hundreds of thousands of distributed and variable renewable resource generators delivering energy services to hundreds of millions of interactive and smart loads. As such, the future grid should and will be significantly different than today's grid.

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* Expanded use of renewable energy is widely considered one key element in a strategy to mitigate emissions and hold projected temperature increases at an agreed-upon level. Other low-carbon elements include, but are not limited to, greater efficiency, land-use management, nuclear energy, and fuel-switching. This report focuses specifically on integrating larger quantities of renewable energy into the nation's electrical grid.

The drivers of change are diverse. The future smart grid will need to address:

- Increasing spatial and temporal complexity of the grid, as stochastic renewables penetrate a grid that was deterministically planned.
- Moving large quantities of renewable energy over long distances reliably.
- Strengthening aging infrastructure for reliability and cost-effective power delivery.
- Controlling power flows.
- Managing grid congestion near large urban centers.
- Dealing with millions of interactive and responsive smart loads.
- Reducing power losses.

The transformation of the future grid will be extensive and will affect generation, demand, delivery, and operations.

Broad Context and Background for Priority Research Directions (PRDs)

An inexorable increase in demand for electric energy has been driven not only by ongoing population and economic growth, but also by the coming electrification of transportation and the need to transport vast amounts of renewable energy to load centers. Therefore, our clean energy technology future requires that we substantially strengthen and expand the fundamental infrastructure of the electric power grid. Furthermore, improving control of power flow in the grid is critically important to enabling more efficient allocation of grid resources and to secure the grid against a growing variety of instabilities and disturbances. Expansion and control will be essential to (1) relieving the grid congestion that today limits economic exchange of electric power, and (2) achieving a more efficient marketplace. There is a major opportunity for significant efficiency improvement in the grid itself, but an even greater imperative is to increase the capacity of existing transmission rights-of-way and develop new underground transmission technology that can circumvent or mitigate difficulties in siting and permitting of new facilities. Figure 7-2 shows the conceptual impact of high-temperature superconductor underground direct current (dc) cables in reducing siting requirements for long-distance transmission of large power from remote renewable sources to load centers.

The following PRDs identified at the Workshop are critical to enabling new technologies needed to address these grid requirements.

High Performance and Reliability of Power Electronic Materials. When the electric grid was invented at the end of the 19th century, alternating current (ac) electricity delivery won over dc because of two enabling technologies: transformers and circuit breakers. By transforming voltage, transformers enabled long-distance transmission of electric energy with low losses; circuit breakers provided an essential safety measure and provided the ability to switch circuits at

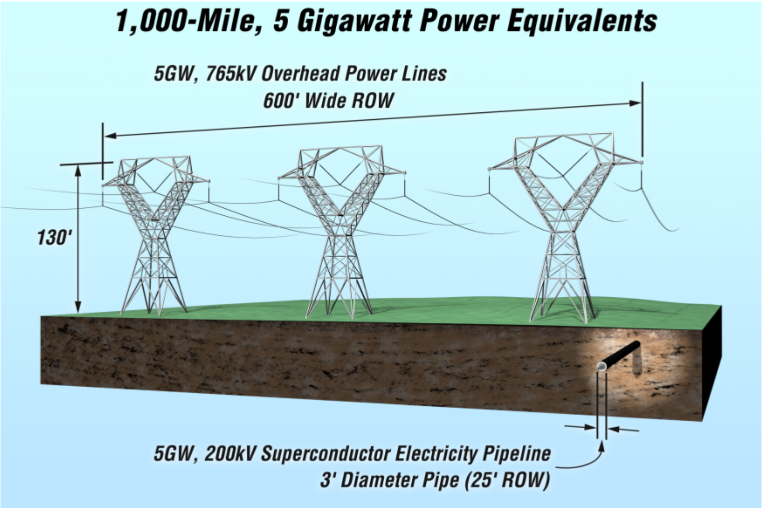

Figure 7-2 Schematic right-of-way (ROW) comparison between conventional high-voltage (HV) overhead and high-temperature superconductor dc cable pipelines. Source: American Superconductor.

high voltage. The invention and development of semiconductor materials and devices have enabled high-power power electronics to perform both of these functions and added additional control over the flow of electricity. Transformers provide the ability to convert ac current at one voltage to a different voltage. Power electronics permit the conversion of ac to ac (transformation), ac to dc (rectification), dc to ac (inversion), and dc to dc (chopping).

Except for the circuit breakers, today's high-voltage ac electric systems do not and cannot control the flow of power; rather, the flow of power is passive and dictated by Kirchhoff's laws. Various types of power electronic devices and systems have been invented to provide the ability to control the flow of energy on the high-voltage electrical network, but their applications have been limited by economics and performance. New materials and devices are needed to enable cost-effective use of power electronics on high-voltage networks. In particular, wide bandgap materials that permit single devices to control current flows at higher voltages with high efficiency could make power electronics affordable and enable efficient tools to control and manage electricity. Some, like silicon carbide, are already known, but need further understanding and improvement to achieve widespread application. New materials are also needed; importantly, they must be practical materials. An enormous amount of new science is needed to design these materials and develop the knowledge of how to fabricate them into practical devices.

High-Temperature Superconductors for the Grid. The ability to deliver large amounts of energy from remote resources to population centers is increasingly limited by the availability and expense of obtaining rights-of-way for overhead transmission lines. A more affordable means of delivering electricity through ultra-high-power (5 gigawatt [GW] or higher) dc underground cables would dramatically improve the situation. The new high-temperature superconductors offer this option, yet have been limited by their cost and performance. A major increase in current carrying capacity could help enable this cable technology. New scientific understanding is needed to create and control the interaction of material defect sites with flux-carrying superconducting vortices and, hence, increase critical current in practical magnetic fields.

In urban areas, overhead transmission has become next to impossible, and conventional underground cables are limited by the crowded existing infrastructure under city streets. Here too, high-temperature superconductors provide a unique solution, because they offer high power density, and because they emit no heat or electromagnetic fields into their surroundings, allowing cables to be placed in close proximity to other underground infrastructure. High-temperature superconductors provide an important new current limiting functionality: if current exceeds a so-called critical current, the superconductor suddenly changes into a resistor, suppressing the current flow. This is of great importance in dealing with the steadily increasing fault currents in large urban networks, which threaten grid stability and safety. High-temperature superconducting technology can be applied not only to cables, but also to transformers, generators, and standalone fault current limiters. All of these applications require the materials advances described above.

Insulating Materials with Improved Dielectrics and Thermal Properties. Lack of space for overhead transmission lines in congested population centers, along with opposition to their construction, forces transmission to move underground. Current properties of underground cables limit the distance underground cables can transmit electricity without expensive compensation for their capacitance. New insulating materials with better dielectric and thermal properties could greatly improve the situation. Yet dielectric properties of many new materials have not been characterized, and novel nanoparticle composites, which promise a major breakthrough, are largely unexplored. Systematic efforts to search for and characterize better-performing materials could result in new underground cable technology, permitting greater use of underground transmission and reducing electricity delivery congestion. Studies of dielectrics at cryogenic temperatures are also essential to enable dc high temperature superconductor cables described in PRD #2.

New Composite Materials for High-Temperature Low-Sag Overhead Transmission. Substantial economies could be achieved today by reducing transmission congestion. The risk of system instability such as occurred in the August 2003 power blackout in the northeastern United States would be mitigated by low-sag overhead conductors (sag intersecting tree growth was an initiating cause of the blackout). Current carrying capacity of existing overhead transmission lines needs to be increased, while not increasing weight or sag caused by thermal expansion from resistive heating at high power. While lower-sag overhead conductors have recently been developed, new composite conductors could offer a major further advance. The scientific challenge is to invent or discover such new conductors, along with feasible fabrication techniques and material properties, which are applicable in large-scale manufacture, all at an affordable price. This requires

…… … we need deeper and more integrated and systems based understanding of grid structure and dynamics. Storage, demand management, and peaking generation are all tools that can be deployed to create a better grid. Understanding the synergies among them and their optimal deployment through data collection, analysis, and deployment is a task we are only beginning to attend to through programs underway in the Department of Energy."

Steve Koonin, Under Secretary for Science, U.S. Department of Energy
December 10, 2009 Testimony before Senate Committee on Energy and Natural Resources Committee

scientific investigation and breakthrough discovery or invention of new macro- and nano-scale solutions.

Systems Issues

In addition to the above PRDs directed to materials and chemistry, a number of fundamental systems-level issues deserve serious attention (see the statement by Under-Secretary Koonin, sidebar). These issues can be addressed within the wider scope of the U.S. Department of Energy Office of Science.

While the grid of the future is expected to be smarter and more robust, it will also be far more complex. The future grid will have hundreds of thousands of variable renewable resource generators, in addition to hundreds of millions of interactive and flexible loads. Wind and solar generation will add far greater uncertainty than the present uncertainty in load. Addressing the increasing spatial and temporal complexity of the grid will require a transformational change from deterministic planning and operation to real-time response based on stochastic theory and modeling. Deeper and more integrated systems-based understanding of the dynamics of the grid of the future is needed.

Understanding — through modeling and simulation — the increasing complexity in both planning and operating the grid requires a major advance in fundamental theory. The scientific challenge is to appropriately model and simulate very large-scale non-linear dynamical systems that include a mixture of variable types (e.g., continuous, discrete, stochastic) representing both physical and economic phenomena, while dealing with uncertainty in data.

The research direction starts with creating a comprehensive and unified theory of large-scale dynamical systems that can be validated experimentally, and incorporates the inherent non-linear complex systems nature of the evolving electric power system.

Another scientific challenge is to develop means for high-bandwidth/low-latency data collection in wide-area networks, along with non-linear and stochastic control algorithms based on high-speed processing. Fast, high-dimensionality/non-linear stochastic control algorithms/software do not exist for real-time decision making. Research directions include investigating hierarchical stochastic optimization and control, parallel computing for stochastic control, ultra-fast screening and reduction of data without loss of critical information, and enhanced visualization of the grid to improve decision making.

The potential impact of this basic research on modeling of the grid system is in providing new means to achieve a robust and resilient power delivery system with a much higher level of dynamic control than is possible today. Grid losses will be reduced, voltage instabilities and blackouts avoided or mitigated (saving billions of dollars in societal cost impacts), the need for new lines reduced, and asset utilization improved.

Other Research Directions: Transformers, Refrigerators, Cryostats

An interesting opportunity to enhance transformer performance comes from new magnetic materials, taking advantage of novel properties of nano-granular materials.

Major improvements in capacity, efficiency, and reliability of cryogenic refrigerators for the 30 to 77 kelvin (K) temperature range are critically important for the new generation of superconductor power equipment. For most of these applications, refrigeration powers of 50 watts (W) to 10 kilowatts (kW) are required. One of the most serious scientific challenges limiting progress in large regenerative cryocoolers of the Stirling, pulse tube, and Gifford-McMahon types is understanding flow non-uniformities, especially in large systems, that lead to significantly decreased efficiencies. Thermoacoustic and other fluid dynamic effects play an important, but as yet, unexplored role. Large regenerative cryocoolers currently have efficiencies of only about 10 to 15% of their theoretical Carnot limit. In large systems, achieving an efficiency of 30% or more of the Carnot limit would transform the operation of the grid through its impact on superconductor power equipment, but this requires basic research on the fundamentals of thermoacoustics as well as the fluid dynamics of steady flow.

Other issues that need to be addressed in fluid dynamics and thermoacoustics include understanding the transition of turbulent and jetting flow into uniform oscillating flow, the non-linear effects on jet-driven heat transport to the cold end of pulse tubes, and the effect of the viscous boundary layer on Rayleigh streaming. Improved physical and computational fluid dynamics models are needed to provide quantitative results for loss mechanisms, along with improved flow visualization techniques for oscillating flow at cryogenic temperatures. Investigation of fluid flow and dynamics in rotating frames is also of importance for use of rotation for pumping. Another set of issues concern energy conversion in activating the fluids and gases involved in cryogenic systems. To develop fundamentally new ideas for pressure oscillators such as linear motors, compressors, and expanders, it is necessary to understand the relationship between magnetic energy density and current density with fluid energy density for increasing efficiency and power density. Scaling and stability limits in large resonant machines need to be defined. It would also be desirable to develop means of direct conversion of electrical energy to fluid energy and vice versa, without moving mechanical parts.

New insulation materials and geometries are also highly desirable, to enable use of non-vacuum environments to reduce cost and increase reliability; vacuum-based insulation is prone to single-point failure. This could include investigations of foams and nano-scale geometries (films or particles) as phonon blockers to reduce the thermal conductivity of composites.

III. PRIORITY RESEARCH DIRECTIONS

A. PRD #1. High Performance and Reliability of Power Electronic Materials

1. Problem Statement

Today's high-voltage ac electric power grid does not control the flow of power, which is dictated rather by Kirchhoff's laws: electricity follows the path of least impedance. But with ongoing demand growth leading to grid congestion and increasing fault currents in urban areas, and with the need for higher efficiency and transport of large amounts of renewable power long distances to load centers by dc transmission, new control strategies and the ability to convert between ac and dc cost effectively are urgently needed. Semiconductor power electronic devices and systems have been invented to do this, but their application has been limited by economics and switching capabilities and losses. Practical new materials and devices are needed to enable cost-effective and efficient use of power electronics on high voltage networks.

2. Executive Summary

The electric power grid has an urgent need for more cost-effective power electronics to provide new flexibility in controlling power flows, especially in grid-congested urban areas, and new options for ac-to-dc conversion enabling efficient dc transmission of large amounts of renewable power to load centers. The keys to such enhanced power electronics are wide bandgap semiconductors with higher voltage capability, lower switching losses, higher reliability, and higher junction temperature capability. The scientific challenge is to understand loss and failure mechanisms in known materials like silicon carbide, and to identify and develop new materials with even higher potential. This requires research in areas such as the origin of defects in large area wide bandgap devices, identification of localized heating and failure mechanisms, understanding of reliability and thermal cycling of metal-insulator interfaces, and exploration of new systems like chemical-vapor-deposited boron-doped diamond. The impact of such research would be the development of more cost-effective power electronics to revolutionize the stability and efficiency of the electric power grid and open up wide use of high-efficiency dc transmission, including the effective transport of renewable energy from remote sources to distant load centers.

3. Context and Background for PRD #1

When the electric grid was invented at the end of the 19th century, alternating current electricity delivery won over direct current because of two enabling technologies — transformers and circuit breakers. Transformers permitted the transformation of voltage and enabled long-distance transmission of electric energy at high voltage, by minimizing current and losses proportional to the square of the current, while circuit breakers provided an essential safety measure and the ability to switch circuits at high voltage. The invention and development of semiconductor materials capable of switching high power have enabled power electronics to perform both of these functions and add additional control over electricity flow in the grid. Power electronics permit the conversion of ac to ac (transformation), ac to dc (rectification), dc to ac (inversion), and dc to dc (chopping). This flexibility makes power electronics one of the keys to a future smart grid.

In modern high power systems, these conversions are performed with silicon-based semiconductor switching devices such as diodes, thyristors, and transistors. Consumer electronics typically contain ac/dc converters (rectifiers) handling tens to hundreds of watts; in industry, the most common application is the variable-speed drive that is used to control induction motor speed, with power ratings of a few hundred watts to tens of megawatts.

Use of switching converters has expanded dramatically since the late 1950s ,with the invention of the semiconductor transistor and, in particular, the subsequent development of the silicon controlled rectifier or thyristor, which replaced the earlier mercury arc tube with much faster switching speed, lower losses, and significantly better operating reliability. The rapidly increasing voltage (up to 10 kilovolts [kV]) and current rating of thyristors together with various power transistors made increasingly high-voltage and -power applications possible, with excellent reliability and high conversion efficiency. Thyristors paved the way in the 1970s for the development of the Static VAR Compensator (SVC) for reactive power compensation and voltage support of ac transmission lines. Subsequently, the technology was extended to series capacitive line compensation by the development of the Thyristor-Controlled Series Capacitor (TCSC). Self-commutated dc-to-ac switching converters, using gate turn-off thyristors or high-power bipolar transistors, made possible the development of advanced compensators and power flow controllers, such as the Static Synchronous Compensator (STATCOM), the Static Synchronous Series Compensator (SSSC), the Unified Power Flow Controller (UPFC), and the Interline Power Flow Controller (IPFC). Today, the functioning of modern manufacturing, transportation, and electric utility industries would be unimaginable without the use of these electronic switching converters.

The Insulated Gate Bipolar Transistor (IGBT), youngest member of the high-voltage switch family, is already widely used. The IGBT's current flow is conveniently controlled through a 15-volt (V) high-impedance voltage source, enabling control of high currents with very low control power and high switching speed. Despite these advances, there are serious limitations to the power electronic technology available today, especially for high-power applications such as connecting high voltage dc power lines to the ac grid. Foremost among these limitations is cost. This arises in part from the limited voltage capability of the devices, with 10 kV thyristors at the high end and most IGBTs used today operating below 1 kV. This leads to large series strings of devices constituting valve-to-switch high voltages, often above 100 kV, in addition to many parallel devices handling high currents, creating enormous system complexity and cost. Efficiency is another major issue, with considerable power lost in large ac-to-dc or dc-to-ac power electronic converter stations, leading to costly thermal management problems. High switching speed is also desirable to enable pulse-width modulation and minimize harmonics, and to avoid bulky passive components, but the limited voltage capability of silicon IGBTs, which have the needed switching speed, limits their use in higher-power applications. As a result, controllers like the UPFC, very desirable to utilities for directing power flows, are installed in only two sites in the United States, and high power dc lines — much desired for long-distance power transfer — are rarely used, except for very long runs like the Pacific Intertie, because of the huge cost of the dc-to-ac converter stations.

4. Industry Needs

The future grid is likely to include many sources of alternative energy, such as wind, solar, and fuel cells, as well as energy storage devices such as flow batteries, compressed air, plug-in hybrid cars, and conventional batteries and capacitors. With power flowing in both directions, two major pieces of power electronics will be required: (1) high-speed power converters, which transfer power between low-voltage solar, fuel cell, and wind generators; and higher-voltage distribution and transmission networks on the grid, and (2) fast-acting solid-state circuit breakers to rapidly connect or disconnect the intermittent distributed sources of power from the grid.

In recent decades, to address the limitations of silicon-based power semiconductors, wide bandgap semiconductors such as silicon carbide have been attracting considerable attention for high-voltage, high-power, and high-temperature applications, owing to superior material properties enabling higher-speed switching, operation above 15 kV, and lower conduction losses in the on-state compared to silicon power switches. This means that high-voltage wide bandgap power switches could support direct interfacing of converters and enable cost-effective transmission-level dc-ac conversion — a game changer in terms of both technology and economics.

A focus has been silicon carbide, whose wide bandgap (3.26 electron volt [eV] vs. 1.12 eV for silicon), high-breakdown electric field (2.2 megavolts per centimeter [MV/cm] vs. 0.25 MV/cm for silicon) and high thermal conductivity (4.9 watts per centimeter [W/cm] vs. 1.5 W/cm for silicon) are all superior to traditional silicon-based systems. These features promise silicon carbide IGBTs/diodes with a dramatic reduction of on-state and switching losses and high operation temperature greater than 175°C. To achieve major impact with silicon carbide, however, module reliability needs to be improved, costs brought down with higher yields, and the voltage range extended further. New materials such as boron-doped diamond promise even better performance.

In summary, the industry need is for a new generation of power electronic devices capable of significantly higher voltages (15 kV or more) and currents, with much higher efficiency and switching speed, reduced failure rates, and higher operating temperatures (100° to 200°C or higher). This implies the need for improved high-power semiconductor materials, including improved silicon carbide and new wide bandgap semiconductors like boron-doped diamond.

5. Scientific Challenges

Achieving improved operating characteristics of power electronics requires scientific understanding of mechanisms generating defects in large area devices, which cause localized heating and/or failure. The present state of the art is commercially available silicon carbide wafers with less than 3 micro-pipes over an entire 100-millimeter (mm) (4-inch) wafer. Active device epitaxial layers 1 to 100 micrometers (μm) thick can be grown with fewer than 0.5 defects per square centimeter (cm^2), which implies that an approximately 50% yield is possible for 1-cm^2 devices as has indeed been demonstrated. The density of 1-c screw dislocations has been reduced below 10^3 cm^{-2}, which results in less than 1 microampere (μA) leakage current in 1-cm^2 devices. Furthermore, basal plane dislocation density has been reduced to below 2 cm^{-2}, resulting in relatively stable bipolar devices. In order to enable silicon carbide material for economic operation above 15 kV, lower defect density and understanding of operational failure or device degradation induced by material defects are critically important.

The scientific challenge is understanding the defect structure, dynamics, and failure modes of silicon carbide, and identifying and developing new materials with even more promising band gaps, switching speed, electrical losses in the on-state, defect formation, and failure modes.

6. Research Directions

1. Improve existing power electronic materials such as silicon carbide.
    - Extend the limits of defect-free large area wide bandgap materials. In collaboration with industry, conduct failure analysis studies, including coordinated microscopy and transport characterization on state-of-the-art large area samples to identify the origin of performance limits, possibly confirming the role of specific defects such as screw, basal plane, and threading-edge dislocations, and identifying new mechanisms of defect formation and their roles in device failure. Next, the origin and control of these defects need to be understood in the context of deposition and growth conditions.
    - Extend the limits of high-voltage performance in bipolar devices. In bipolar devices, enhancing performance for high voltage and power requires increasing epitaxial layer thickness, which is currently limited by decreasing carrier lifetime. Mechanisms of lifetime loss with increasing thickness need to be studied, with correlated microscopic studies of possible defects. Once the defects are identified, control methodologies need to be developed by studying defect density under systematically controlled deposition conditions.
    - Understand and control localized heating development and failure mechanisms in wide bandgap semiconductors. Failure mechanisms under thermal cycling need to be identified, with particular attention to the interfaces between metallic and insulating layers.
2. Evaluate and begin development on new advanced power electronic materials like gallium nitride and boron-doped diamond grown by chemical vapor deposition [7].

7. Potential Impact

A new generation of power electronic materials will enable lower cost, higher output, more reliable operation with current-control, and ac-to-dc conversion functionality that will transform operation of the future electric power grid from passive to active. Cost-effective high-voltage dc-to-ac power converter stations will open up wide applications of efficient dc power links and enable massive dc transmission of renewable energy to distant load centers. More cost-effective medium-voltage power switching and flow controllers will enable wider use of dynamic control of distribution grid power flow, which can mitigate voltage instability, increase grid reliability, manage grid congestion in urban areas, and reduce power losses by effective allocation of power paths through the grid, creating new functionality and billions of dollars in savings.

B. PRD #2. High-Temperature Superconductors for the Grid

1. Problem Statement

The ability to deliver energy from remote wind and solar resources to distant population centers is essential for tapping our abundant renewable resources. Conventional high-voltage dc transmission lines, the preferred option for distances more than a few hundred miles, are challenged by high losses for long lines and the limited availability and expense of obtaining rights-of-way for overhead transmission lines. Within population centers, the availability of the necessary rights-of-way is often particularly restricted. A more affordable and easily permitted means of delivering electricity is urgently needed. High-temperature superconductors offer the promise of this option, yet have been limited by their performance and cost. A major increase in current-carrying capacity in fields at operating conditions is required to enable a broadly viable commercial solution.

2. Executive Summary

Achieving a national goal to reduce greenhouse gas emissions while at the same time meeting anticipated electricity demand growth will be enabled by a stronger and smarter grid, and will require substantial additions of transmission to carry renewable energy resources from remote locations to population centers. In some locations of great natural beauty or dense development, transmission facilities must be built underground. A major advance in the current-carrying capacity of high-temperature superconductors could make underground ac and dc transmission more economic and practical. While the most impactful application of high-temperature superconductors is underground transmission, significant opportunities also exist for more efficient and effective transformers, generators, motors, and fault current limiters. Research directions focus on understanding vortex physics to enhance critical current density in existing and new materials.

3. Context and Background for PRD #2

The utility industry has an urgent need for underground transmission lines with lower cost and enhanced reliability to mitigate grid congestion near large urban centers, with reduced rights-of-way and the ability to move large quantities of renewable energy over long distances reliably. Utilities need to upgrade and hybridize the aging infrastructure to maintain reliability and cost-effective power delivery, and reduce power losses.

The ability to deliver energy from remote resources far from population centers is limited by the availability and expense of obtaining rights-of-way for overhead transmission lines. Within population centers, the availability of the necessary rights-of-way is often particularly restricted. A more affordable and easily permitted means of delivering electricity is urgently needed. High-temperature superconductors offer the promise of this option, yet have been limited by their performance and cost.

4. Industry Need

High-temperature superconductor power equipment — cables, transformers, generators, and fault current limiters — meet broad utility industry needs, and significant prototypes have been demonstrated. But to achieve competitive cost-performance, significant improvements over existing wire performance are still required, chief among these being a major increase (at least a factor of two) in high-temperature superconducting current-carrying capability under operating conditions, as well as a reduction in cost. For high-temperature superconductor ac cables, current limiters, and transformers, performance in liquid nitrogen at 77 K and in fields up to 0.1 tesla (T) is required; for dc cables, the field requirement increases to almost 1 T. High-temperature superconductor generators and motors operate in a conduction-cooled environment of 30 to 40 K in fields in the 2 to 4 T region (see also requirements for wind generators in *Chapter* 9 *[Panel 8]*). High-temperature superconductor technology could lower electrical losses in transformers, generators, and motors, and importantly — reduce their size and bulk, lowering costs.

5. Scientific Challenges

Lowering superconductor wire cost is largely an industrial challenge. The scientific challenge resides in enhancing the wire's capability to carry electric currents with zero resistance, i.e., without energy dissipation. The critical current density (the maximum current density that can be carried with no dissipation) is determined by the material's microstructure. Magnetic fields penetrate superconductors in nanosized discrete strings called vortices. Electric currents exert forces on the vortices, and in a crystallographically perfect material, arbitrarily small currents induce vortex motion, generating dissipation. To obtain zero resistance, it is necessary to preclude the vortex motion. This occurs when the material has structural inhomogeneities or defects that locally reduce the vortex energy, thus "pinning" them by producing a force that counteracts the force of the current as long as it does not exceed the critical current density.

Pinning centers form naturally in the fabrication or can be artificially created to increase the critical current density. Their effectiveness depends in a complex way on their size, shape, composition, and distribution. Progress has been made in increasing the critical current density by introducing non-superconducting second phases via chemical routes (see Fig. 7-3) that are more suitable for industrial-scale production, in some cases involving self-assembly of the second phases into nanorods or planar aggregations of nanoparticles. However, presently, these efforts are mostly based on semi-empirical approaches or even simple trial and error.

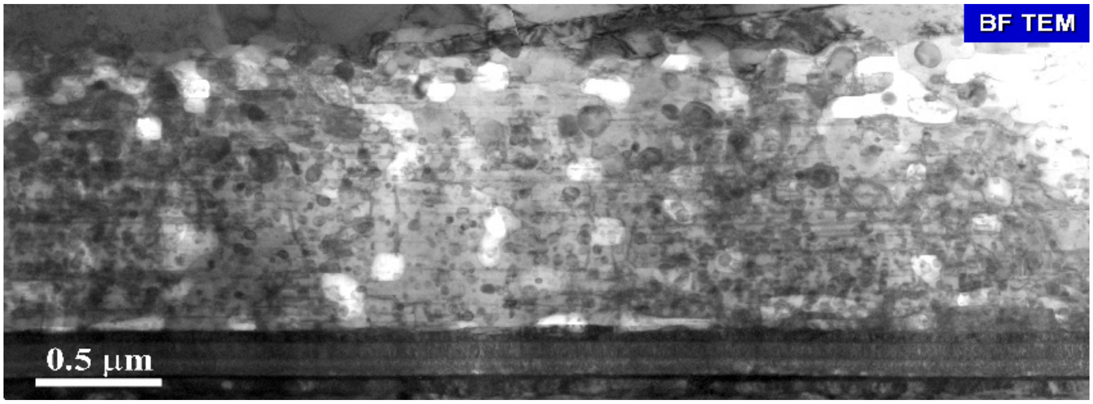

Figure 7-3 A cross-sectional bright field (BF) transmission electron microscopy (TEM) image of a state-of-the-art yttrium barium copper oxide (YBCO) high-temperature superconductor layer in a coated conductor, with a critical current of 450 A/cm-width at 77 K. Three ~75- nanometer (nm)-thick buffer layers are seen at the bottom separating the YBCO from the texture nickel tungsten (NiW) substrate. Visible in the YBCO are planar stacking faults, nanoprecipitates (dark dots), and porosity (white areas), all of which contribute to the complex pinning landscape controlling current density.
Source: T. Holesinger, Los Alamos National Laboratory.

Although the critical current density resulting from some simple "model" defect distributions is reasonably well understood, moving beyond current phenomenological approaches to increase the critical current density will require dramatically improving fundamental knowledge of vortex pinning and dynamics.

A basic question is, what is the maximum critical current that could be obtained by introducing the "ideal" distribution of defects? According to present knowledge, at low magnetic fields we should be able to obtain a critical current density as large as the depairing current density, the absolute maximum limit (different for each superconductor) set by the physics of superconductivity. However, even in the best cases (coated conductor and niobium titanium [NbTi] wires) only 25 to 30% of that value has ever been reached. If methods to increase pinning close to the theoretical limit can indeed be found, then factors of three increases in critical current density (implying a similar reduction in system costs) could be achieved. Even more complex is the situation at high temperatures and in the presence of large magnetic fields, where the simultaneous interactions of many vortices with many defects must be considered, resulting in a many-body problem that far exceeds the current understanding of the subject. Designing superconductors that can operate efficiently at higher magnetic fields and temperatures is required for many applications. An additional problem is posed by thermal fluctuations in vortex matter, which are orders of magnitude larger in the cuprate high-temperature superconductors than in conventional low-temperature superconductors, due to a combination of two factors: the small superconducting coherence length (which is directly related to the high superconducting transition temperature) and the large crystalline anisotropy. Fluctuations have two main detrimental effects. First, they induce a melting of the vortex matter into a liquid phase, which occurs at a characteristic temperature dependent irreversibility field $H_{irr}(T)$ where the critical current density goes to zero, so that the vortex liquid lacks dissipation-free current carrying capability. Second, they provide a certain probability for vortices to escape from the pinning centers, even for current densities smaller than the critical current density (an effect called flux creep), resulting in a reduction of the effective critical current density and in residual dissipation below the critical current density. Both negative effects increase with increasing anisotropy; thus the discovery and/or design of less anisotropic high-temperature superconductors would be highly beneficial.

At the present time, coated conductors based on $YBa_2Cu_3O_7$ (yttrium barium copper oxide [YBCO]) films are the commercial choice for power grid applications. The progress made in recent years in improving their properties by optimization of buffer layers, introduction of second phases, chemical doping, and control of processing conditions has been enormous. Presently, coated conductors have such good texture that the grain boundary current-limiting problem has been either eliminated or significantly reduced, and the critical current density in typical operating conditions is one order of magnitude higher than 10 years ago. However, large pinning improvements, particularly in magnetic field, are still needed for many applications. Thus, work needs to focus on building the scientific knowledge base for these existing and very promising materials. New high-temperature superconductor materials, such as the pnictide family of iron-arsenic-based compounds, continue to be discovered, and their vortex properties deserve exploration to determine whether they could have favorable properties for application.

6. Research Directions

1. *Identification and modeling of vortex pinning mechanisms.* This will involve combined experimental and theoretical efforts, both in well-controlled “model systems” and in realistic pinning microstructures. A wide range of temperatures and fields should correspond to those required for applications. Industry’s main interest now is to improve existing $YBa_2Cu_3O_7$ materials. For a general understanding of vortex physics, studies should include a variety of materials, even if they do not have immediate technological relevance. Most of the obtained knowledge will also be applicable to yet-to-be-discovered superconductors. This work will require new methods to achieve three-dimensional mapping of the pinning landscape.

2. *Reduction of the detrimental effects of thermal fluctuations, for reduced flux creep and higher temperature operation*. The most straightforward approach would be to discover and/or engineer superconductors with lower anisotropy. An alternative possibility is to pin the vortex liquid phase, which will require studies up to very high magnetic fields, both to determine the anisotropy and to understand vortex matter under extreme conditions.

3. *Understand the electronic and vortex properties of multiband superconductors*. The recently discovered iron-arsenic-based superconductors open up many possibilities for novel vortex physics and fundamental mechanisms of superconductivity. Two attractive characteristics of pnictides are their large upper critical fields and their multiband electronic structure. The bands may have opposite anisotropies and result in almost isotropic effective properties, which could address the thermal fluctuation problem. The chemically simpler two-band superconductor magnesium diboride (MgB_2) can also provide useful insight.

4. *Atomic level microstructure control of high-temperature superconductor films on textured substrates for higher pinning and reduced grain boundary current limiting*. The improvement in the properties of cuprate high-temperature superconductor films by manipulation of their microstructure has been very successful and must be continued. However, more fundamental approaches aimed at controlled engineering of the pinning landscape at the atomic level, as well as understanding and controlling superconductor/buffer and superconductor/inclusion interfaces, are necessary to produce significant further progress. This work is preferably done on existing coated conductors based on $YBa_2Cu_3O_7$ materials to accelerate the impact on practical applications. This will also require new tools, including methods to fabricate high-temperature superconductor films on textured substrates with atomic level control to engineer the vortex-pinning landscape.
5. *Discovery of new high temperature superconductors by design or serendipity*. In parallel with the incremental improvement of known materials, the search for superconductors with better properties, stronger pinning, higher field and temperature operation, lower anisotropy, and higher superconducting transition temperature must be pursued.

7. Potential Impact

The impact of successful development of higher-performance and lower-cost superconductors is to enable a host of new high-temperature superconductor power equipment that will revolutionize the electric power grid. Benefits include increased power transmission capability and grid reliability, reduced transmission cost, effective incorporation of renewable energy, elimination of energy delivery bottlenecks, and reduction of losses.

C. PRD #3. Electrical Insulation Materials for Power Cables

1. Problem Statement

Significant economic benefits accrue if conventional underground ac cables could be made available with increased power-carrying capacity and with capacitive charging length limits doubled or more without the need for reactive power compensation. High-current-capacity dc cables and superconductor cables are needed for long-distance transmission systems, such as those collecting and transmitting power from large-scale remote distributed wind farms and solar plants to load centers. Improved dielectric materials for electrical insulation of the cable conductors are a key technology required to enable these benefits.

2. Executive Summary

Lack of space for overhead transmission and distribution lines in congested population centers, along with esthetic opposition to their construction, forces power links underground. The distance underground ac cables can transmit electricity is limited without expensive compensation for cable capacitance. New materials with better dielectric and thermal properties would enable broader use of underground transmission and reduce electricity delivery congestion. To meet this need, dielectric properties of new materials should be significantly improved, exploring novel nanoparticle composites as one promising opportunity. Dielectric performance and reliability at liquid nitrogen temperature must also be tested and improved if necessary, especially for dc cable application, where little is known.

3. Context and Background for PRD #3

Grid expansion to fulfill future electric energy load growth will continue to meet with opposition from interest groups affected by the right-of-way of overhead lines. Thus, future expansion in such areas will require underground burial of medium and high voltage cables.

Load growth demands either higher-power-carrying-capacity cables within the same corridors, or new corridors that are often difficult to obtain even underground. Higher capacity can be enabled by dielectrics and other cable components with higher-temperature capability, up to 130°C or more, allowing higher thermal dissipation, hence higher current. Superconductor cables are the ultimate path to much higher capacity.

AC cables are limited in length of individual runs because of the need to charge the cable capacitance each cycle, resulting in a significant phase shift in voltage and current, and so, they require expensive reactive power compensation. This limiting “charging length” is now typically 20 to 30 miles, and an industry need is for cables with significantly lower capacitance, enabling a doubling of the capacitive charging limit. This will significantly simplify underground cable installations and enable their use more broadly in the electric power grid. Superconductor cables have inherently low capacitance because of their compact size for a given power rating.

DC cables do not have this capacitive limit problem. The major limitation for dc cables is the cost of ac-dc conversion at the terminals, which require distances of several hundred miles to become economically viable. The power delivered by conventional dc cables can be increased by higher operating temperatures of improved dielectrics.

4. Industry Need

A common theme in all these grid issues is the industry need for improved dielectrics. Cross-linked polyethylene in various forms is the most widely used distribution and transmission cable insulation today for underground cable voltages ranging from a few hundred volts to over 500 kV. New dielectric materials with lower dielectric constants and high thermal capability will enable the cable technology needed to address industry needs. Dielectrics are also a critical element of superconductor cables, both ac and dc.

5. Scientific Challenges

The scientific challenge is to develop or improve dielectric materials for electrical insulation of the cable conductors. Dielectric materials with twice the design stress of today’s polymeric-based insulation materials are needed. This will allow thinner insulation and, thus, increased power density and improved thermal conductance, enhancing thermal performance. The lowest possible dielectric constant will reduce the cable capacitance; materials with a relative dielectric constant of less than two are desired. The dielectric material should also have a high temperature capability, preferably at or above 130°C, with high thermal conductivity.

Well-characterized dielectric materials for cryogenic temperatures are critical for superconductor high capacity transmission cables. Little is known about the properties and long-term reliability of dielectrics in the 77 K temperature range, at which high-temperature superconductor power transmission cables operate, either under ac or dc operation. For the cryogenically cooled ac cables, the dielectric constant and the dielectric losses in the material are important factors. For the cryogenically cooled superconductor cables, the dielectric losses become very important to minimize since they require a factor of 20 more power to remove these losses to room temperature from a liquid-nitrogen-cooled cable.

For dc cable insulation, an important material characteristic is reduction or elimination of the space charge accumulation in the material and interfaces as a result of the unidirectional voltage supplied, since this can lead to dielectric breakdown. This is important for both room temperature and superconductor cables.

6. Research Directions

Research in dielectrics for medium- and high-voltage applications has largely been neglected in the United States for decades. It thus appears that the dielectric properties of many new materials have not been characterized. A research program to meet the challenges should start with a quantitative identification of candidate materials. Many of these materials may not have been considered for use as electrical insulation in cables, overhead lines, or transformers. Thus, gaps in the characterization of the candidate materials exist and must be filled. Material candidates for both extruded insulations (such as the majority of the polymeric-based cables today), and for tapes in thick- and thin-film applications, should be included.

A promising research direction for dielectric materials involves nanoparticle fillers. Nanoparticles have been shown to increase the dielectric strength of dielectric materials and reduce statistical scatter in the breakdown voltage (e.g., see Fig. 7-4). Several classes of these nanoparticles should be explored for improved dielectric and thermal insulation characteristics. How these particles are affected by the material processing, such as the extrusion process or tape manufacturing, needs to be explored. Atomic-level control of the nanoparticle fillers, their dispersion, and the interfacial interactions with each other and the dielectric material matrix must be understood in order to achieve reliability at industrial scale and in low-cost manufacturing processes. For dc cables, dielectrics with low or no space charge accumulation at the conductor/dielectric interface are important.

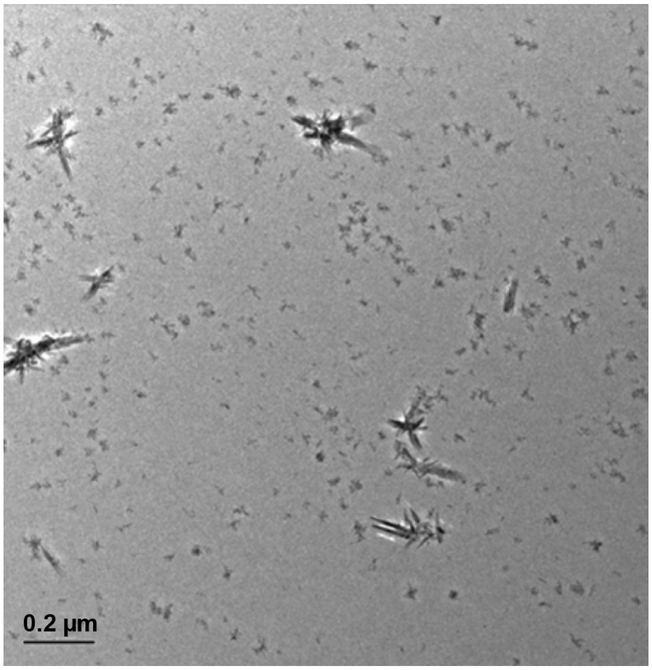

Figure 7-4 Crystalline TiO_2 nanoparticles and nanofibers in a polyvinyl alcohol amorphous matrix. Dielectric breakdown properties are significantly improved with the addition of the nanoparticles. [7]. Source: E. Tuncer, Oak Ridge National Laboratory.

Characterizing and mitigating breakdown processes of standard and novel cable insulation materials in the 77 K range, under ac and dc conditions, is an important area, where little is known. These include the standard partial discharge tests under ac and dc conditions, plus basic impulse-level lightning impulse testing. Correlation of results with the microstructure can reveal mechanisms of partial discharge. Aging tests need to be devised for both ac and dc operation to assure long-term reliability.

7. Potential Impact

The results of dielectric research will enable higher-capacity underground transmission cables with a high power density due to smaller and lighter insulation and two to three times longer-distance ac transmission with reduced need for expensive reactive compensation and forced cooling. The reduced cost and broader applicability of underground links will solve many of today’s transmission bottlenecks. For dc transmission, materials with no space charge accumulation at the conductor/dielectric interface are key to achieving a future scenario of an interconnected dc regional/national grid, enabling high-capacity transport of remote renewable energy to load centers.

D. PRD #4. New Materials for Overhead Conductors

1. Problem Statement

An increasingly high-capacity and capable power transmission system is urgently needed to meet load growth and to transport renewable energy from distant sources to load centers. A major element in this system is the overhead power transmission line, and more capacity in these lines will be needed. To avoid the costly and time-consuming development of new rights-of-way, enhanced power capacity in existing corridors is highly preferable. One path to such higher capacity is through new overhead conductors with low sag and higher current capability.

2. Executive Summary

Reduced transmission congestion could provide substantial economies. Ongoing load growth demands more transmission capability, and large amounts of electricity generated from remotely sited renewables will need to be moved efficiently to population centers. Consequently, the pressing need is for increased current-carrying capacity of existing overhead transmission lines. The challenge is to increase current-carrying capacity of overhead transmission lines while not increasing weight or the sag caused by thermal expansion with increasing temperature. The scientific challenge is to develop new advanced metallic or composite conductors, fabrication techniques, and material properties that can be maintained in large-scale manufacture and at an affordable price. Systematic scientific investigation and breakthrough discovery of new composite and nano-scale solutions need to be pursued.

3. Context and Background for PRD #4

Some 50 million people were left without power on August 14, 2003, when a transmission line near Cleveland sagged close enough to a tree to spark an arc that tripped relays and took the line out. This simple event led to cascading failures and voltage collapse, which resulted in a massive blackout of a large fraction of the midwestern, northeastern, and mid-Atlantic United States, and parts of Canada. The common overhead transmission line is essential technology of modern society, but it is, for the most part, the same technology that has been used for decades. Blackout stories, at both a local and regional scales, point to the urgent need to begin upgrading this country's aging electricity delivery infrastructure, and particularly, the overhead transmission line system, to reduce the risk of blackouts and assure reliable electricity delivery.

Different forecasts of U.S. energy growth all point to the need for substantially increasing the miles of high-voltage transmission lines. One major need will be to access wind power in the Great Plains and transport the wind energy over thousands of miles to the eastern United States. In addition, new lines will be needed to meet load growth around the country. However, the challenge of obtaining rights of way for new overhead transmission lines is becoming more severe.

As an existing transmission line carries more current, it becomes fully "loaded" and reaches a limit beyond which operation increases the risk of a failure in the system. A thermal limit occurs at sufficiently high line current that its temperature exceeds its thermal rating, causing the line to sag to below safety limits or possibly become permanently damaged by plastic deformation. The line can be dynamically rated to gain at least 10% or more capacity, but eventually, either a new line will have to be built in parallel to the existing line, or the conductor in the existing line will have to be replaced with a higher-capacity conductor. Given the vast network of overhead rights-of-way already established, the cost-effective solution for most needs is to upgrade existing lines for higher capacity while maintaining other key conductor performance features like low sag.

4. Industry Needs

The specific industry needs related to overhead transmission conductors are as follows:

1. Enable delivery of larger power over existing overhead transmission lines.
2. Reduce power losses.
3. Increase utilization of existing transmission assets and rights-of-way.
4. Improve ability to handle high currents during faults to prevent cascading failures.
5. Improve corrosion resistance of overhead lines.
6. Achieve longer life and reduce susceptibility to wind-driven vibration failure of overhead lines.

5. Scientific Challenge

The path to meeting these industry needs requires new and improved conductor materials with (1) low-cost premiums over existing conductors, (2) similar weight, (3) excellent corrosion resistance, (4) lower electrical resistance, (5) lower thermal expansion, (6) increased short-circuit current tolerance, (7) less susceptibility to wind-driven vibration failure, and (8) higher emissivity than existing conventional conductors.

A first step in this direction has been the invention, development, demonstration, and commercialization by 3M of an aluminum conductor alloyed with zirconium to improve thermal and electrical conductivity. The wrapped core strands contain aluminum oxide fibers embedded in high-purity aluminum, forming a wire called “aluminum conductor composite reinforced” or ACCR. This fiber-reinforced metal matrix has strength equivalent to steel, with mass density similar to aluminum, but with less thermal expansion than steel and strength retention at high temperatures. This new conductor demonstrates that the search for new materials and concepts for overhead conductors is promising. Apart from ACCR, little basic work has been done in this topic.

Specific goals are to achieve handling twice the current of the most-widely used existing conductors (ACSR) with little line sag at temperatures above 200°C, and reduce line losses by at least 10% while operating at voltages up to 765 kV, with a nominal premium in cost over existing conductors.

6. Research Directions

A first step is to understand the limits of existing overhead conductors like ACSR and annealed aluminum conductor steel supported (ACSS) with trapezoidal wire cross-section, as well as the recently introduced ACCR conductors. From this understanding, a target set of improved electrical conductivity, mechanical, weight, thermal, and chemical properties could be developed for further advances.

Two promising classes of materials for investigation are composite and nanomaterials. There is a huge range of composite materials, including metal-metal and metal-ceramic combinations. The composites could include components with complementary desirable properties, such as Invar alloys with zero or even negative thermal expansion that will counter the tendency of lines to sag as they heat.

In the class of nanomaterials, carbon nanotubes could enable a major breakthrough. These lightweight materials have extraordinary strength — greater than steel. The so-called armchair configuration of carbon nanotubes is metallic with conductivity superior to copper [8]. The possibility of stranding nanotubes together to form a cable has already been demonstrated, though not yet with the predominance of metallic configurations [9].

Multiple challenges, however, face the nanotube concept. The first is producing nanotubes in sufficient quantity and at low-enough cost; this industry is rapidly developing. The second more scientific challenge is to separate out the nanotube configurations that have sufficiently low conductivity, since of the many possible topological configurations, most are insulating or semiconducting rather than metallic. Self-selecting schemes for metallic conformations could exploit their higher conductivity. A third challenge is developing a practical method for stranding such nanotubes together into a long cable. Developing contacts and understanding the conductivity between neighboring nanotubes will also be critical. Nanotubes can also be doped to modify properties, and the effect of purposeful as well as accidental impurities needs to be understood. Appropriate impurities, for example, might convert the preponderance of semiconducting nanotube configurations into conducting ones.

7. Potential Impact

Improving overhead conductor performance will allow better utilization and increase power transfer capability for new lines and retrofits to existing lines, to allow greater power transfer in new or existing transmission corridors, lowering the cost of transmission service, and better utilizing transmission assets. More renewables can be delivered to customers over existing transmission lines, and the environmental impact of new rights-of-way can be eliminated or mitigated. Electrical losses on the transmission and distribution system in the United States are approximately 8%. The current investment in transmission and distribution has a replacement value on the order of several trillion dollars. Reducing losses and deferring upgrades could save tens of billions of dollars, and so, could be key to achieving a more capable and reliable grid that meets future energy needs.

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Chapter 8: Panel 6 — Advanced Solid State Lighting
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I. EXECUTIVE SUMMARY

An astounding 22% of total electricity or 765 terawatt-hours (TWh) generated annually in the U.S. is used solely to generate lighting [1]. Approximately half of this electricity (321 TWh) is consumed by incandescent and halogen sources, though these sources account for merely 12% of all of the lighting produced each year due to their overall low efficiency of 8-20 lumens per watt (LPW). Solid-state lighting (SSL) based on inorganic light-emitting diodes (LEDs) and organic light-emitting diodes (OLEDs) has the potential to deliver energy saving with system efficiency exceeding 150 LPW, superior lifetime, and equivalent or better light quality relative to the entrenched technologies.

To harness the SSL potential, the LED system efficiency has to be improved by a factor of two while simultaneously decreasing the SSL lamp cost by a factor of 10, to less than $10 per 1000 lumen. Reaching these targets can be accelerated by basic research supporting technology development in the following areas:

- Discovering narrow-line wavelength converters across the red and green spectral range that provide high quantum efficiencies,
- Understanding and overcoming the factors limiting the LED efficiency at high power density and operating temperatures, and
- Uncovering the fundamental mechanisms of the molecular interactions among OLED hosts, guests, interfaces, impurities, contacts, and the environment that limit their reliability.

II. PANEL REPORT

Role of Advanced Lighting in the National Energy Picture

The cost and energy efficiency of lighting technology are crucial elements to solving this nation's energy crisis. Energy consumption for all lighting in the United States is about 22% of the total electricity generated in the country. Based on existing technology, the amount of site electricity consumed for lighting is expected to increase ~1% per year by 2025, to 972 TWh

(Fig. 8-1). The traditional lighting sources of the installed base are among the least energy-efficient technologies in use today. The incandescent bulb produces approximately 5% light and 95% heat. Even the more efficient fluorescent and high-intensity discharge lamps when inserted into luminaires produce only 40-80 LPW useable light and, therefore, convert to light only up to ~25% of the consumed electrical energy. Providing more efficient light sources to the market would offer a major savings in electricity demand and the potential for considerable cost saving to consumers and businesses, which collectively spend approximately $58 billion per year to light their homes, offices, streets, and factories.

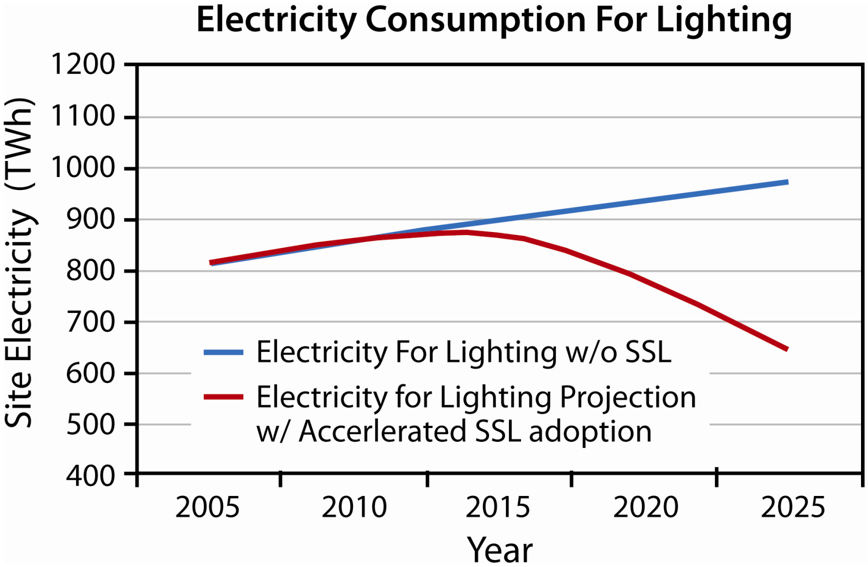

Figure 8-1 Forecast of the electrical energy consumption for lighting through 2025 with and without SSL. Source: [2].

Solid-state lighting offers the potential to save up to 326 TWh in electricity consumption by 2025 (Fig. 8-1), provided that significant adoption (>50%) can be achieved. The two main factors that affect reaching these energy savings are the efficiency of the SSL lamps themselves and their market price. Other factors, such as manufacturing-driven product consistency, market education, and incentives are essential as well, but act only as accompanying elements.
Figure 8-2 shows the SSL performance roadmap that, based on existing market models, would enable the required adoption. Solid-state lighting should exceed 150 LPW at a color rendering index of 76-90 for general lighting. Simultaneously, the cost for these systems needs to be below $5 for a 1000-lumen lamp equivalent. Given these aggressive but achievable performance targets, the cost savings associated with the reduced electricity consumptions can amount to >$22 billion annually from the commercial, residential, and industrial sectors.

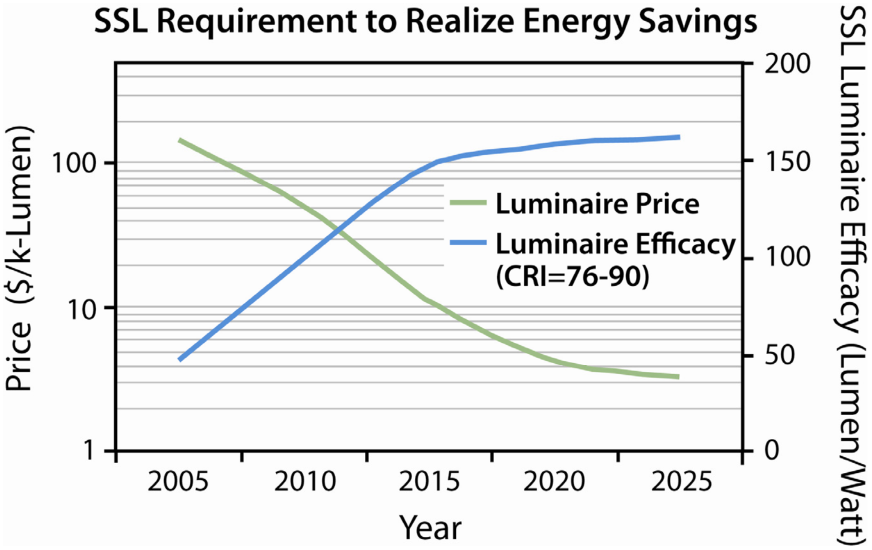

Figure 8-2 Forecast of SSL performance and cost requirements to meet the ultimate energy savings challenge via universal SSL adoption. Source: [2].

Status of Present and Ultimate Industrial Technology Deployment

Inorganic LEDs are emerging as a viable solution in applications like commercial indoor and outdoor lighting. Aside from the product efficiency, additional factors like product lifetime, quality of light, and associated lifecycle cost savings are driving the adoption from currently small levels at relatively high incremental rates. Street and retail lighting are application examples (Fig. 8-3). However, the cost for providing high-quality LED light to the broader commercial and residential market is still too high by about a factor of ten. Furthermore, current LED lights for indoor use operate at just 50-65 LPW, and the efficiency must be improved by more than two times.

The adoption of OLEDs in general lighting is currently barred by their lifetime, with the degradation of the blue-emitting molecules being the limiting factor. Although used in small displays, the OLED luminance and reliability requirements for general lighting are higher by about an order of magnitude compared with those of the small displays, imposing even steeper reliability challenges. Furthermore, OLEDs have yet to demonstrate the scaling of low operating voltages to large areas without tradeoffs in efficiency and cost.

Fundamentally, there is no barrier for either LED or OLED systems to reach efficacies of 160-200 LPW. The semiconductor industry has proven in other sectors that high-efficiency device properties can be scaled to large production volumes and reach required cost reduction, provided associated scientific challenges in device and materials fabrication processes are met. For both LEDs and OLEDs, significant breakthroughs at the scientific and technology development frontier are needed to close the existing gap between the current product status and the performance called for in the SSL adoption roadmaps.

Figure 8-3 (Left) The Chicago Center for Green Technology uses indoor LED lighting to reduce its energy demand for lighting by 64%, freeing the building's solar panels to produce electricity for other uses. Source: Eric Taub, New York Times, 2/29/2009. (Right) With superior color quality and lifetime and high lumen output, LEDs are the emerging technology for the next generation of outdoor lighting. Source: Luminus Devices, Inc.

Background for the Priority Research Directions

Basic SSL research can be an effective catalyst for ongoing technology development. Although the LED industry is starting to commercialize lighting products, significant fundamental problems remain unsolved, which, if not addressed, could cause SSL to level off at lower performance levels. This would stretch out SSL adoption and reduce the total energy savings. The Workshop Panel on Advanced Lighting recommends focusing the basic SSL research toward improving the SSL device efficiency, uncovering the mechanisms limiting device efficiency and reliability, and developing solutions to achieve high device efficiency and reliability under high power density and application-relevant operating conditions.

Addressing and solving these problems would benefit the technical community as a whole and benefit the competitiveness and independence of the U.S. economy in the emerging SSL industry. The research directions outlined below are high risk and complement the primarily applications-oriented industry investments. They, therefore, offer the potential for the proposed basic SSL research to have an impact over the next five years and beyond.

The efficacy of SSL systems needs to improve compared with today's performance levels by a factor of two. The spectral power distribution covering most of the entire visible range is critical for socially acceptable lighting, while LEDs produce only a single wavelength and usually require converters to achieve the desired output wavelengths; however, converters further lower efficiency. Identifying SSL emitter sources that operate efficiently in preferred regions of the visible spectrum can help close this efficacy gap. Practical choices of wavelength converters are limited to a few yellow/green/red-emitting materials. Consequently, industry has adopted a technologically viable approach that uses blue-emitting LEDs and one or two broadband wavelength conversion materials. Identifying wavelength converter hosts that show potential for high-efficiency, narrow-line [full width at half maximum (FWFM) < 50 nm] emission, in particular, in the red spectrum range, can lead to significant SSL efficiency advances. Alternatively, uncovering pathways that overcome the lack of red and green direct-emission

LEDs that operate efficiently at high power densities and temperatures would represent a breakthrough with significant application potential. Figure 8-4 illustrates a spectral simulation of the efficiency benefits that can be derived by flexibly placing such narrow-line solid-state emissions across the visible spectrum.

While efficient LED operation of up to 200 LPW has been demonstrated in the laboratory [3], the efficacy of practical LED systems is more than 50% lower due to the high power density and high temperature required in practical applications (Fig. 8-5). Blue-emitting LEDs based on gallium nitride (GaN) are used in virtually all such LED systems. Despite the progress in LED research, the following rather fundamental questions remain unanswered:

- Why does the external quantum efficiency of blue-emitting GaN LEDs decrease with increasing operating current density and temperature? This is the phenomenon often called "droop."

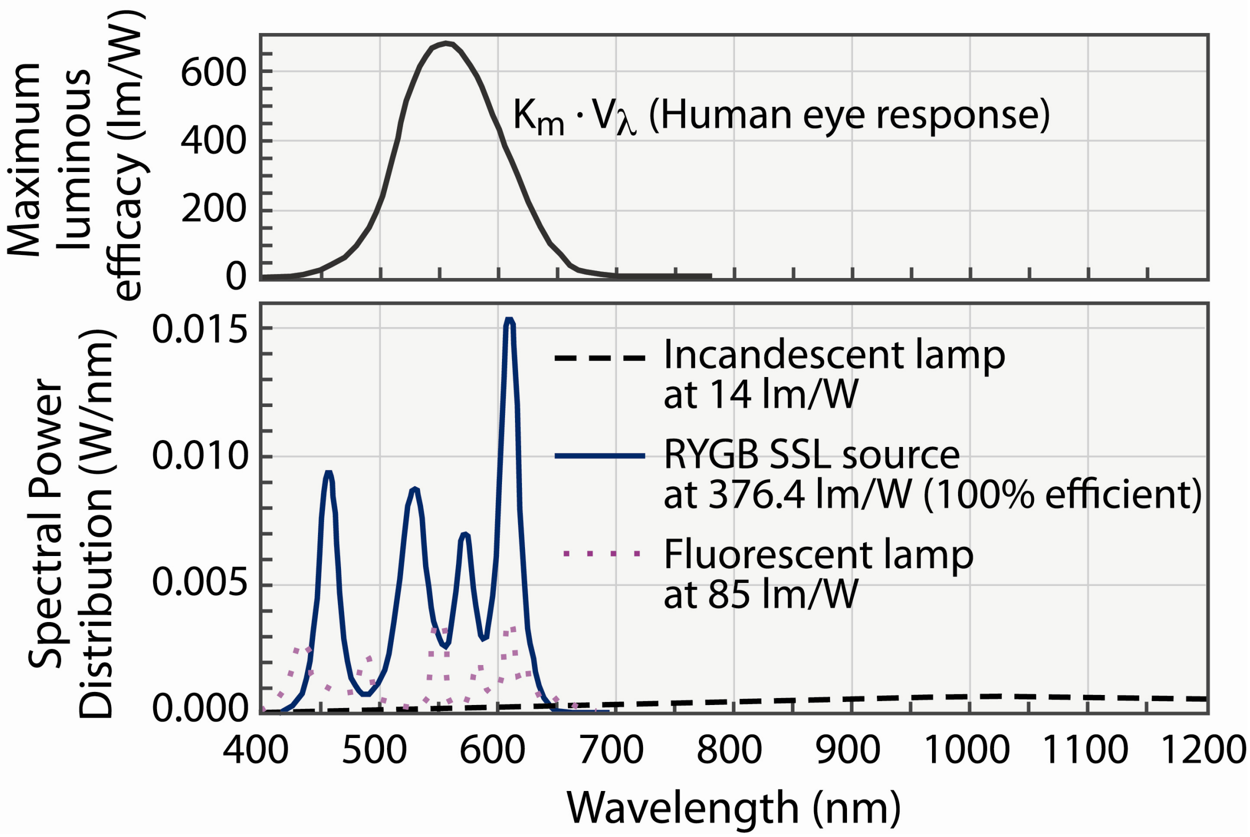

Figure 8-4 Simulated example for creating efficient, high light quality white SSL emission with narrow-line emitters spaced across the visible spectrum. Combining direct emission and wavelength-conversion approaches can enable >160 LPW SSL devices. Source: J. M. Philips, P. E. Burrows. Office of Basic Energy Sciences, Basic Research Needs for Solid-state Lighting. May 2006. http://www.sc.doe.gov/bes/reports/files/SSL_rpt.pdf

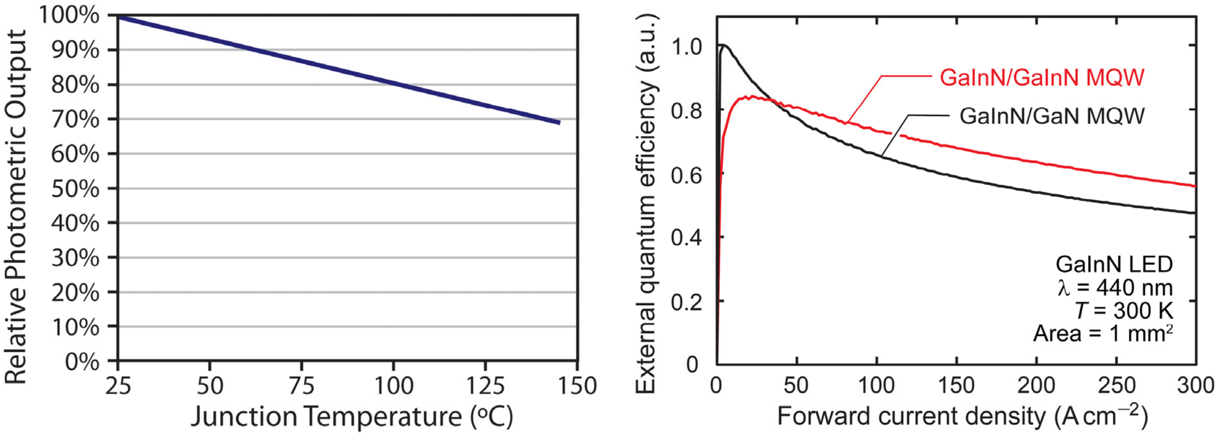

Figure 8-5 Efficiency "droop" of LEDs at high operating temperature (left) and high current density (right). This phenomenon is not understood at the fundamental level and, if overcome, could result in an ~50% efficiency improvement. Sources: (left) LED Luminaire Design Guide, Cree, Inc, 2007 [4] and (right) Xu et al, Appl Phys Lett 94, 011113 (2009) [5].

- Can the temperature sensitivity of red direct emitters be mitigated in conventional phosphide or other materials without compromising LED efficiency?
- What are the processes limiting the efficient radiative recombination in green-emitting LEDs, and how can they be overcome?

Similar to LEDs, OLEDs have shown that efficient white light generation is possible. However, in contrast to LEDs, a perhaps more fundamental scientific challenge is extending the applicability of OLEDs to general lighting applications: can the reliability of blue-emitting OLED materials, in particular, under high luminance operating conditions, be improved and, simultaneously, can the system losses associated with the operating resistance and voltage be reduced? Current predictive methods for materials selection and screening do not provide sufficient insight into the limiting mechanisms with regard to device reliability and efficiency.

Building the scientific foundation to break through these performance-limiting problems is of paramount importance to enable widespread adoption of SSL throughout the residential and commercial sectors. Engineering solutions so far have not provided the answers. Based on these fundamental challenges for LED and OLED approaches, three priority research directions (PRDs) were defined and are described below. These PRDs overlap many of the PRDs developed in the earlier report on basic research needs for SSL, although they focus more on understanding existing materials and their modifications for nearer term impact rather than on searching for new materials that could ultimately provide new generations of SSL systems.

Description of the Priority Research Directions

White Emission through Wavelength Conversion. The efficient generation of white light from solid-state emitters is limited to blue-emitting LEDs that are combined with broad yellow- and red-emitting wavelength converters. One path toward fabricating white light sources with a significantly higher efficiency and high color quality involves use of emission sources that operate at high wall plug efficiency throughout the entire visible spectrum.

Current wavelength-converter hosts for solid-state white light generation are limited by the broad emission spectrum (typical FWHM ≥100 nm), the low quantum efficiency due to the intrinsic material properties or immature fabrication methods (in particular, in the red spectral range), thermal efficiency quenching under operating conditions, the excitation capability by blue light sources, and in some cases, the chemical stability of the host materials under the high temperature and high light flux density of SSL systems. In the red spectral range, there would be significant payback in LED efficiency with the availability of a red wavelength converter with FWHM ≤ 50 nm. Development of high-efficiency direct emitters in the 530-630 nm range that operate at high temperatures and power densities has been so far elusive as well.

The focus of this research direction is to identify and explore novel classes of wavelength conversion materials that offer significant potential to provide <50-nm wide emission in the 530-630 nm range under 430-460 nm excitation, with the 590-630 nm emission range being of particular interest. Novel inorganic host lattices, quantum dots structures, or organic/inorganic hybrid materials should be investigated. The basis of this work should be fundamental research leading to an improved understanding of the ability to tailor the excitation of inorganic and hybrid hosts to the desired wavelengths and high quantum efficiencies, and providing insights into mechanisms for reduced temperature quenching and catastrophic degradation of converter materials.

Successful outcomes of this PRD would be proof-of-concept demonstration of the following:

- Wavelength conversion materials with an external quantum efficiency of ≥90% at operating temperatures of ≥ 100°C under 430-460 nm excitation, and
- Wavelength conversion materials, based on red or green solid-state emitters, that exhibit a wall plug efficiency of ≥50% at ≥100°C.

High-Efficiency Visible Solid-State Emission at High Current Density and Temperature. Blue-emitting GaN LEDs is an emerging SSL system, but still suffers from an efficiency drop at high operating power densities (“droop”). The underlying mechanism for the droop is not understood. Furthermore, the use of LEDs in lighting systems imposes high-temperature operating conditions, which for blue-emitting and even more for red-emitting LEDs, leads to an additional reduction of the device efficiency. Experimental, theoretical, and empirical approaches have provided no satisfactory explanations for some of these device limitations. Several mechanisms (Auger recombination, polarization, interplay of defects, strain, carrier transport, recombination, etc. [6-9]) have been proposed but not yet proven. Furthermore, an improved understanding of the mechanisms limiting the thermal efficiency of nitride and phosphide semiconductors could identify pathways toward improving the temperature-dependent efficiency quenching.

One aspect of this research direction is to focus on developing analytical tools and methods that shine a light on the operating behavior of nitride LEDs (e.g., nano-current imaging). The LED operating behavior is critically linked to device design and materials quality. Therefore, it is recommended that these fundamental studies be conducted on state-of-the-art devices and materials to increase the probability that the insights gained on efficiency droop will have practical application. Such devices and materials can be obtained from industry and highlight the need for direct Basic Energy Sciences (BES)-industry collaboration. To complement this analytical approach, further research should be conducted in materials fabrication processes to better understand the impact of the crystal structure, point defects, and lattice defects. This work should further be coupled with efforts toward development of improved device design tools and simulation methods and their experimental verification.

Successful outcomes of this PRD would be:

- An experimentally verified root cause of the efficiency droop at high current densities in blue-emitting LEDs,
- A proof-of-concept demonstration of a blue-emitting LED with 60% wall plug efficiency operating at a current density of 150-200 A/cm^2, and
- A proof-of-concept demonstration of blue-, green-, or red-emitting LEDs with a thermal degradation of the external quantum efficiency by < 20% between room temperature and 150-200°C.

OLED Materials and Structures for Reliable, Color-Consistent, High-Luminance Emission. The reliability of OLEDs, in particular, blue-emitting materials, has been one of the fundamental obstacles toward their commercialization for lighting applications. The reliability challenge is, in part, due to the energy of the blue emission approaching the bond energy of functional elements within the organic molecule. So far, predictive materials selection and screening methods for promising blue-emitter materials have proven insufficient and largely ineffective for narrowing down the search. This shortcoming leaves materials scientists largely to trial-and-error methods. At the OLED device scale, fundamental understanding is lacking on the interactions between different materials and at their interfaces. The relationship between the materials morphology at the nanometer scale and the device reliability and performance of, for example, contacts is also unknown.

Therefore, this PRD is focused on gaining a fundamental understanding of molecular interactions among OLED hosts, guests, interfaces, impurities, contacts, and their environment. The objective is to uncover the reactive mechanisms that limit OLED device reliability and then to identify molecular design rules and device fabrication routes that improve device lifetime and performance under the high excitation conditions required for lighting applications.

Successful outcomes of this PRD would be:

- The demonstration of material and device models that link the molecular design and structural device properties to expected degradation behavior and device properties (e.g., efficiency, contact resistance),
- The proof-of-concept demonstration of a blue-emitting OLED with predicted 10,000-hr lifetime, and

- The proof-of-concept demonstration of white light OLED with the same predicted lifetime at a luminance of 10,000 candela per square meter (cd/m^2).

III. PRIORITY RESEARCH DIRECTIONS

A. PRD #1: High-Efficiency, Visible, Solid-State Emission at High Current Density and Temperature

1. Problem Statement

Solid-state lighting based on inorganic LEDs has the potential to reduce lighting electricity use in the U.S. by one-third. This is the annual equivalent to saving the output of forty-four 1000-megawatt power plants or the greenhouse gas emissions of 47 million cars [10]. To achieve the necessary SSL system efficacies, some fundamental problems in LED technology must be solved. In particular, the efficiency decrease ("droop") at high current density and high temperatures currently limits the performance and cost of today's SSL systems.

2. Executive Summary

Solid-state lighting has the potential to deliver energy-saving lighting solutions with system efficacies exceeding 150 LPW, superior lifetime, and equivalent or better light quality relative to the entrenched technologies. To harness SSL potential, LED efficiency has to be improved by a factor of two while simultaneously decreasing the SSL lamp cost by more than a factor of ten, to less than $5 per delivered 1000 lumens. Significant breakthroughs in LED technology are needed to close the existing gap between the current product status and the performance called for in the SSL adoption roadmaps. Reaching these targets can be accelerated by basic research to understand and overcome the factors limiting the LED efficiency at high power density and operating temperatures.

3. Industry Need

Solid-state lighting systems should exceed 150 LPW at a color rendering index of 76-90 for general lighting. Simultaneously, the cost for these systems needs to be below $5 per 1000-lumen lamp equivalent. Current LEDs for indoor use operate at just 50-65 LPW; so the efficiency must be improved by more than a factor of two, along with a factor of ten cost reduction.

Fundamentally, there is no barrier for SSL systems to reach efficacies in the 160-200 LPW range. Efficient LED operation of up to 200 LPW has been demonstrated in the laboratory [3], but the efficacy of practical LED systems is more than 50% lower due to the requirements of high power density and high operating temperature in applications (Fig. 8-5). This efficiency decrease at high current density and high temperature strongly affects the cost for SSL systems.

The Droop forces tradeoffs among total luminous flux, efficiency, LED count, and cost. For example, as current density is increased, a LED chip can produce more light output at the same cost, thereby requiring fewer LEDs per system, though this comes at the expense of lower efficiency. To achieve high flux and efficiency, more LEDs are run at a lower current density, thus increasing costs. Solving the droop issue would significantly lower the cost of SSL systems while simultaneously maintaining a high operating efficiency.

Although the LED industry is starting to commercialize lighting products, significant fundamental problems remain unsolved. These problems, if not addressed, could cause SSL to level off at lower performance levels. Reaching expected efficiency and cost targets can be accelerated by basic research uncovering mechanisms and developing solutions for high device efficiency and reliability under high power density and application-relevant operating conditions. Engineering solutions so far have not given the answers.

4. Scientific Challenges

Despite the progress in LED research, the following fundamental questions remain unanswered:

- Why does the external quantum efficiency of nitride-based LEDs decrease with the operating current density?
- Can the temperature sensitivity of red direct emitters be mitigated in conventional phosphide or other materials without compromising the LED efficiency?
- What are the processes limiting the efficient radiative recombination in green-emitting LEDs, and how can they be overcome?

The GaN-based LEDs, the light source of choice in emerging SSL systems, still suffer from an efficiency drop at high operating power densities. Furthermore, the use of LEDs in lighting systems imposes high-temperature operating conditions, which for blue-emitting and even more for red-emitting LEDs based on aluminum indium gallium phosphide (AlInGaP) leads to an additional reduction of the LED efficiency. Experimental, theoretical, and empirical approaches have provided no satisfactory explanations so far. Several mechanisms such as Auger recombination, polarization, interplay of defects, strain, and carrier injection have been suggested by the scientific community [6-9], though a consensus on the mechanism remains elusive.

Additionally, an improved understanding of mechanisms limiting the thermal efficiency of nitride and phosphide semiconductors could identify pathways toward improving the temperature-dependent efficiency quenching. The AlInGaP material system has indirect band-gap minima, which fundamentally limit temperature insensitivity, especially at short wavelengths. In addition, poor carrier confinement due to the small band offsets is a major source of the temperature sensitivity. In the GaN system, the source of the temperature dependence is not well understood; possible mechanisms include Auger recombination, carrier overflow, and recombination dynamics.

Lastly, an improved understanding of efficiency loss in the green region of the spectrum, the so-called “green gap,” is needed to provide efficient green-emitting LEDs. The GaN-based LEDs show high external quantum efficiencies in the blue region. Longer wavelength devices, achieved by increasing the indium concentration in the InGaN active region, show a considerable drop in efficiency, which could be attributed to materials issues such as polarization and strain effects but the dominant cause is still unknown [13]. The AlInGaP-based LEDs, on the other hand, show impressive performance in the red region, but lose efficiency at shorter wavelengths. The direct-indirect band-gap crossover in the yellow-green region provides a clear explanation for this efficiency drop, making their improved performance in the green region far less likely. Unlike AlInGaP alloys, InGaN alloys possess a direct-energy band gap across the visible spectrum and present no intrinsic roadblock to high-efficiency optical emission.

5. Research Directions

One aspect of this research direction is to focus on developing analytical tools and methods that “shine light” on the operating behavior of nitride LEDs (e.g., nanocurrent imaging), and on carrier lifetime measurements as a function of current level. In LEDs, the operating behavior is critically linked to the device design and materials quality. Therefore, we have recommended that these fundamental studies be conducted on state-of-the-art devices and materials to increase the probability that the insights gained on droop will have practical application. Such devices and materials can be obtained from industry and highlight the need for direct BES-industry collaboration.

To complement this analytical approach, further research should be conducted on materials fabrication processes to better understand the impact of the crystal structure, point defects, and lattice defects. This work should be coupled with efforts toward development of improved device design tools and simulation methods and their experimental verification.

Successful outcomes of this PRD would be:

- An experimentally verified root cause of the efficiency droop at high current densities in state-of-the-art blue-emitting LEDs,
- A proof-of-concept demonstration of a blue-emitting LED with 60% wall plug efficiency operating at a current density of 150-200 A/cm^2,
- A proof-of-concept demonstration of a green-emitting LED with 50% wall plug efficiency operating at a current density of 35 A/cm^2, and
- A proof-of-concept demonstration of blue-, green-, or red-emitting LEDs with a thermal degradation of the external quantum efficiency by < 20% between room temperature and 150-200°C.

6. Potential Impact

Solving the droop problem would give LED lighting products higher efficiency at a fraction of the current cost, enabling broad market penetration, with major electricity savings and consequent environmental benefits. This solution would also benefit the competitiveness and independence of the U.S. economy in leading the emerging SSL industry. Cost savings associated with the reduced electricity consumption can amount to >$22 billion annually combined among the commercial, residential, and industrial sectors. The research directions outlined above are high risk and complement the primarily applications-oriented industry investments. They offer the potential for the proposed basic SSL research to have an impact over the next 5 years and beyond.

B. PRD #2: White Emission through Wavelength Conversion

1. Problem Statement

Energy consumption for all lighting in the United States is about 22% of the total electricity generated in the country [1]. Providing more efficient light sources to the market would offer a major savings in demand for electrical energy and also the potential for considerable cost saving to consumers and businesses, which collectively spend approximately $58 billion per year to light their homes, offices, streets, and factories. To achieve the necessary SSL system efficacies, some fundamental problems in LED technology must be solved. Uncovering pathways that overcome the lack of red and green (530-630 nm range) direct-emission LEDs that operate efficiently at high power densities and temperatures would represent a breakthrough with significant adoption potential.

2. Executive Summary

Solid-state lighting based on inorganic LEDs has the potential to deliver energy saving lighting solutions with system efficacies exceeding 150 LPW, superior lifetime, and equivalent or better light quality relative to the entrenched technologies. To harness SSL potential, LED system efficiency has to be improved by a factor of two while simultaneously decreasing SSL lamp cost by a factor of ten, to less than $5 per 1000 lumens. Significant breakthroughs in LED technology are needed to close the existing gap between the current product status and the performance called for in SSL adoption roadmaps. Reaching these targets can be accelerated by basic research supporting technology development to discover narrow-line wavelength converters across the red and green spectral range that provide high quantum efficiencies.

3. Industry Need

The cost for providing high-quality LEDs to the broader commercial and residential market is still too high by about a factor of ten. Furthermore, the efficacy of SSL systems needs to improve compared to today’s performance by a factor of two.

A spectral power distribution covering most of the entire visible range is critical for high-quality, socially acceptable lighting. Since LEDs produce only a single wavelength, they require wavelength converters to achieve the desired white light output. These converters currently lower the overall SSL efficiency significantly.

At this time, the efficient generation of white light from solid-state emitters is limited to blue-emitting LEDs combined with broad yellow- and red-emitting wavelength converters. These current wavelength converter hosts for solid-state white light generation are limited by the broad emission spectrum (typically, FWHM $\geq$ 100 nm), the low quantum efficiency due to the intrinsic material properties or immature fabrication methods (in particular, in the red spectral range), thermal efficiency quenching under operating conditions, the excitation capability by blue light sources, and in some cases, the chemical stability of the materials under SSL operating environments of high temperature and high light flux density.

One path toward fabricating white light sources with significantly higher efficiency and simultaneously high color quality requires emission sources that operate at high wall plug efficiency throughout the entire visible spectrum. In particular, there would be significant payback in LED efficiency with the availability of a red wavelength converter with FWHM $\leq$ 50 nm. Uncovering pathways that overcome the lack of red and green (530-630 nm range) direct-emission LEDs that operate efficiently at high power densities and temperatures would represent a breakthrough with significant adoption potential. Figure 8-4 illustrates a spectral simulation of the efficiency benefits that can be derived by flexibly placing such narrow-line solid-state emissions across the visible spectrum.

4. Scientific Challenges

Fundamental materials challenges remain to improving wavelength conversion for SSL. In particular, can new classes of materials be developed, such as inorganic host lattices, quantum dots, or organic/inorganic hybrid materials, that provide red and green narrow-band wavelength converters that are efficient and thermally stable?

Breakthroughs are needed in red-emitting phosphors to produce white light LEDs suitable for general applications. Virtually all of the red phosphors that have been developed for use in SSL have drawbacks. Currently, these phosphors contain rare earth dopants (Eu^{2+} or Ce^{3+}) in sulfide-, oxide-, or nitride-based host lattices. These dopants emit light due to 5*d*-4*f* transitions. Because the 5*d* orbitals are spatially diffuse, their energy levels depend strongly on the crystal fields of surrounding ions in the host lattice. This sensitivity of the energy levels to the surrounding matrix leads to emission band broadening because of differences in the atomic environments (inhomogeneous broadening) and phonon coupling (homogeneous broadening) [[12]. An undesirable consequence of broad emission is unwanted deep-red emission, to which the eye is insensitive. The broad absorption can also lead to unwanted absorption of green or yellow emission from other phosphors in the mixture, thereby reducing the overall conversion efficiency due to the fundamental Stokes loss associated with the down conversion of light. For these reasons, we believe the development of narrow-band red (and green) emitting phosphors for SSL applications is important.

For high luminous efficacy at device operating conditions, and good color control over a range of operating powers, phosphors must have low thermal quenching. Early red phosphors had either low absorption in the blue-light range (e.g., oxides) or low chemical stability (e.g., sulfides). Research in nitride compounds for Eu^{2+} activators led to the development of a new class of phosphors based on nitridosilicates, which exhibit higher quantum efficiencies, good thermal quenching, and chemical robustness. These comprise the state-of-the-art red phosphors used in the SSL industry today [13]. Unfortunately, the nitridosilicate phosphors still suffer from a broad emission due to the 5d-4f transition and are only a stepping stone until new materials are developed.

5. Research Directions

The focus of this research direction is to identify and explore novel classes of wavelength conversion materials that offer significant potential to provide <50-nm FWHM emission in the 530-630 nm range under 430-460 nm excitation, with the 590-630 nm emission range being of particular interest. Novel inorganic host lattices, quantum dots structures, or organic /inorganic hybrid materials should be investigated. New classes of materials utilizing the narrow band emission of the 4f-4f transitions (such as Eu^{3+} or Mn^{2+} dopants for red phosphors) show potential. In rare earth ions, the electronic *f-f* transitions involve localized electrons in the atomic orbital of the ions, resulting in narrow band emission due to the parity-forbidden 4*f*-4*f* transitions, which are weakly dependent on the crystal field (for example, Eu^{3+} emits at ~610 nm in Y_2O_3, and at ~625 nm in Y_2O_2S) [3].

This fundamental research will lead to an improved understanding of the ability to tailor the excitation of inorganic and hybrid hosts to the desired wavelengths and high quantum efficiencies and will provide insights into mechanisms for reduced temperature quenching and catastrophic degradation of converter materials.

Successful outcomes of this PRD would be:

- The proof-of-concept demonstration of wavelength conversion materials with an external quantum efficiency of ≥ 90% at operating temperatures ≥100°C under 430-460 nm excitation, and
- The proof-of-concept demonstration of wavelength-converter-based red or green solid-state emitters with a wall plug efficiency of ≥ 50% at ≥100°C.

6. Potential Impact

Developing a new class of wavelength converters with efficient, temperature-stable, narrow-band emission in the red and green spectral regions would significantly enhance the competitiveness of SSL, leading to increased market demand and consequent electricity savings for the economy as a whole. It would also benefit the competitiveness and independence of the U.S. economy in the emerging SSL industry. The final result would be a more efficient white light LED with simultaneously high color rendering index – essentially breaking today’s tradeoff between efficiency and color rendering index. Solving significant fundamental technical problems will prevent SSL from leveling off at lower performance levels, stretching out the timeline for SSL adoption and reducing the total energy savings.

C. PRD #3: OLED Materials and Structures for Reliable, Color-Consistent, High-Luminance Emission

1. Problem Statement

Organic LEDs have the potential to enable commercially competitive SSL. However, to achieve the necessary SSL efficacies, some fundamental problems in OLED technology must be solved: most significantly, uncovering the fundamental mechanisms of the molecular interactions among OLED hosts, guests, interfaces, impurities, contacts, and the environmental agents such as oxygen and water that limit their reliability.

2. Executive Summary

Solid-state lighting based on OLEDs has the potential to deliver energy-saving lighting solutions with system efficacies exceeding 150 LPW, superior lifetime, and equivalent or better light quality relative to the entrenched technologies. To harness the SSL potential, the LED system efficiency has to be improved by a factor of two while simultaneously decreasing the SSL lamp cost by a factor of ten, to less than $5 per 1000 lumen. Significant breakthroughs in OLED technology are needed to establish a lighting product capable of meeting the performance called for in SSL adoption roadmaps. Reaching these targets can be accelerated by basic research to understand and overcome the factors limiting OLED reliability at high illumination levels.

3. Industry Need

Organic LEDs have attracted much attention due to the fact they intrinsically emit uniform light, making them excellent diffuse lighting sources. In addition, OLEDs can offer much thinner large-area forms than conventional lighting. Currently, only a few OLED lighting products for general illumination exist in the marketplace. Hurdles to commercialization include improving the efficacy, improving lifetime, and reducing cost. The performance must double from today's laboratory results of 68 LPW for a white OLED panel [14], while scaling to larger area panels [15]. Simultaneously, the cost must decrease.

White light is generated by combining red, green, and blue phosphorescent organic layers in the device. Among the three primary colors, blue is a technical bottleneck for OLEDs since it typically exhibits a lower current efficiency and shorter lifetime than the red and green devices. Today, materials emitting pale blue phosphorescent light have lifetimes of 10,000-20,000 hr at display brightnesses, decreasing substantially as the brightness is increased at least ten-fold for lighting applications. Deeper blues have yet shorter lifetimes. Similar lifetimes are observed for the less-efficient fluorescent dopants used in display applications. This results in differential aging between emission color components of a white light source; hence, the color shifts during the operational lifetime of the source.

4. Scientific Challenges

Organic LEDs have shown that white light generation is possible with an efficiency as high as 102 LPW. However, a more fundamental scientific challenge is limiting the applicability of OLEDs to general lighting applications: Can the reliability of OLED materials, blue in particular, under high luminance operating conditions be improved, and simultaneously, can the system losses associated with the operating resistance and voltage be reduced?

The reliability shortfall is largely due to the energy of the blue exciton, which is electrically formed by injection. When two excitons (or an exciton and an excited state injected charge) collide and annihilate, the resulting excitation can exceed the bond energy of the functional materials (e.g., the dopant and host) in the emitting layer of the OLED. This condition represents a fundamental limitation to the lifetime of blue-emitting organic materials. Predictive materials selection and screening methods for promising blue-emitter materials have proven insufficient to narrow the search for blue-emitting OLEDs. This shortcoming leaves materials scientists largely dependent on trial-and-error methods for seeking appropriate guest-host systems for very long-lived ultra-bright white OLED sources. Alternative approaches to solving this problem may lie in the use of novel molecular solutions, such as dendrimers, unconventional phosphorescent molecules, phosphorescent/fluorescent molecular combinations, and small molecule or polymer systems where guest and host are combined on a single molecular scaffold.

Furthermore, interactions between different materials and at their interfaces are not well understood, and can also serve as a source of degradation at high drive currents used in lighting applications. For example, organic heterojunctions forming boundaries between the emission and injection layers or organic-metal contacts are all subject to degradation under intense excitation. The relationship between the materials morphology at the nanometer scale and the device reliability and performance of contacts is thus still not well understood.

5. Research Directions

The focus of this PRD is the development of a fundamental understanding of the molecular interactions among OLED hosts, guests, interfaces, impurities, contacts, and environmental agents such as oxygen and water. Additionally, the elevated temperatures experienced during operation can accelerate many of these degradation mechanisms, and these effects are not well quantified. The objective is to systematically determine the mechanisms that limit the OLED device reliability, and its dependence on the energetics of the materials and relationship to emission wavelength. Based on this understanding, predictable molecular design rules and device architectures may be identified and fabrication methods may be developed to improve the device lifetime and performance under the high excitation conditions required for lighting applications. A target operating lifetime with less than 10% brightness degradation over 10,000-hr operation at 1000 cd/m^2 is sought.

Successful outcomes of this PRD would be:

- Development of unambiguous physical models for degradation mechanisms, and determination of their relationship to exciton and polaron energetics under different current and thermal load conditions.
- Based on degradation models, development of material models that link the molecular design and structural device properties to the expected degradation behavior and device properties. In particular, guest-host interactions and design of compatible and robust systems are required.
- Development of physical models that clarify degradation mechanisms at organic heterojunctions and at interfaces between organics and contacts. From these models, one should gain insight into appropriate molecular design for use in stable heterojunctions and appropriate metal-organic combinations leading to stable contacts under a variety of excitation and environmental conditions.
- Proof-of-concept demonstration of a blue-emitting OLED with predicted 10,000-hr lifetime at a luminance of 1000 cd/m^2.
- Proof-of-concept demonstration of the use of stable blue-emitting guest-host systems used in combination with stable red and green guest-host systems to form a white-emitting device architecture with minimal color drift and loss of brightness over 10,000 hr at a luminance of 1000 cd/m^2, along with a >150 LPW efficiency at a color rendering index >80.

6. Potential Impact

Developing a new class of blue-emitting OLED materials with efficient, reliable performance would open a competitive solution for SSL, increasing market adoption with consequent electricity savings benefits. It would also benefit the competitiveness and independence of the U.S. economy in the emerging new SSL industry. Although the OLED industry is starting to commercialize a few lighting products, significant fundamental technical problems remain unsolved. Addressing these issues would enable OLED lighting to meet general lighting requirements and service broad market segments.

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Chapter 9: Panel 7 — Biofuels
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I. EXECUTIVE SUMMARY

The manufacture of biofuels has a well-established, commercialized first generation using foodstuffs such as sugars and starches as raw materials, and producing primarily ethanol via fermentive processes. Next-generation biofuels development will focus on non-food feedstocks dominated by lignocellulosic materials. Lignocellulose is not only Earth's most abundant carbon source, it is also highly renewable and provides ample material to generate biofuels. However, lignocellulosics are highly recalcitrant to conversion into biofuels. Several key scientific problems remain which, when solved, will enable optimization of processes now being developed to unlock their stored energy. This study defines three key areas where basic science solutions will pave the way for more efficient second-generation biofuels processes and for more cost-efficient methods of producing petroleum fuel substitutes.

II. PANEL REPORT

Role of Biofuels in the National Energy Picture

Biofuels constitute a broad range of combustible materials slated for use in automobiles, jet engines, diesel fuel, and small engines. Both feedstock sources and processes involved in manufacturing biofuels have numerous possibilities, which are just beginning to be explored.

World energy demand continues to grow rapidly with continued dependence on coal- or petroleum-based sources. The production and use of biofuels holds the promise of meeting a significant portion of the liquid transportation fuel energy needs of the United States as well as globally [1,2]. As shown in Fig. 9-1, rapid production growth is projected. The Energy Independence and Security Act of 2007 projects terrestrial-based biofuels will account for 30% of U.S. demand by 2030, producing as much as 60 billion gallons per year [3]. Aquatic-based crops could add significantly to these figures. "The U.S. Department of Energy has determined that more than 1 billion dry tons of biomass could be sustainably harvested from U.S. fields and forests, enough to displace 30 percent of the nation's annual petroleum consumption for transportation fuels" [4]. The Natural Resources Defense Council has further projected that an aggressive plan to produce lignocellulosic biofuels in the United States could produce

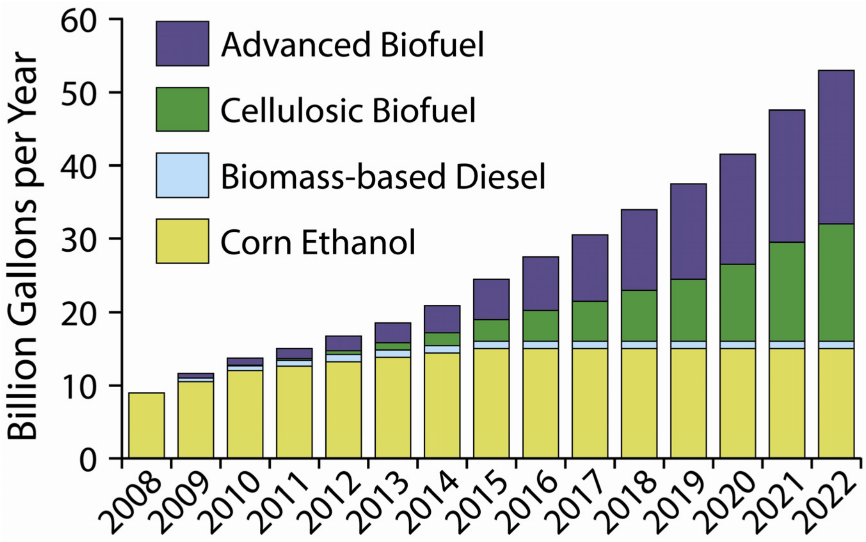

Figure 9-1 The Renewable Fuel Standard in the Energy Independence and Security Act of 2007 calls for a rapid acceleration in the production of cellulosic and advanced biofuels, and a capping of corn ethanol at 15 billion gallons per year. Data from Environmental Protection Agency (http://www.epa.gov/oms/renewablefuels/420f09023.htm#3) and ethanol.org (http://www.ethanol.org/index.php?id=78#Renewable%20 Fuels%20Standard).

the equivalent of nearly 7.9 million barrels of oil per day by 2050, or more than 50 percent of current total oil use in the transportation sector, and more than three times the total Persian Gulf oil imports [5].

Beyond providing a sustainable replacement for oil, biofuels address the global issues of greenhouse gas emissions and the threat of climate change. Widespread use of biofuels will be one of many responses to help drive down the level of atmospheric carbon dioxide in that they hold the promise of carbon neutrality, which other fossil fuel sources cannot attain.

First-generation processes and infrastructure are currently in place producing biofuels, mostly ethanol. However, these operations use feedstocks from readily convertible sources of biomass, which are also food sources: corn, wheat, and sugar, as well as other minor sources. This puts pressure on the food supply, and in addition, food as a feedstock has an unfavorable net energy content compared to non-foods.

The second generation of feedstocks for biofuels is now being developed and holds the promise of being independent of food and hydrocarbon sources by utilizing either purpose-grown non-food crops or waste materials from food production [6]. Source materials for second-generation biofuels include organic materials of photosynthetic origin or their byproducts. Examples include lignocellulosic materials from purpose-grown crops (see Fig. 9-2), waste from the forestry and paper industries, algae, food byproducts, and municipal solid waste with high cellulose content. Lignocellulosic materials are the most abundant sources of carbon known and are completely

Figure 9-2 Purpose-grown biomass feedstock – miscanthus - for second-generation biofuels production. Source: Verenium Corp.

renewable as part of the carbon cycle of plants, namely turning carbon dioxide into less oxidized forms of carbon. In lignocellulose, the main constituents are 5- and 6-carbon sugars as polymers. The monomer sugars are considered in much of the second-generation biofuels processes to be the desired intermediates from which to make fuels.

A third generation will likely evolve through genetic engineering of crops that are designed to be more easily degraded and fermented. An example of the ever-increasing genomic information that will facilitate these efforts is the recent genome sequence of maize [7]. Such engineered materials will be more efficiently processed into fuels but are still in the research stage.

The processes to convert feedstock to biofuels fall into two major categories: those using biological processes such as living organisms or enzymes, and those using thermal and traditional catalytic conversion steps.

The fundamental goal of this and all science efforts in this field is to learn how to convert biomass to the desired fuel products faster and with better control. The technical challenge is driven by emerging new process technologies as well as the complexity of the feedstocks and their relation to the processes. Biomass differs so much in composition and reactivity from fossil fuels that traditional hydrocarbon refining knowledge is inadequate in transformation methodologies. Understanding and developing these processes constitutes the central scientific challenge addressed in this panel report.

Beyond the scientific challenges, there are difficult technological challenges to implementing the production and use of biofuels. Logistics problems include moving biomass to the conversion process location while maintaining a positive energy balance. Since the materials are generally acquired as solids, they cannot be transported by pipeline, and, hence, the use of fuel for harvesting and transport is currently required. In addition, harvested materials may have significant variation due to factors such as storage times and methods, weather and soil conditions, and adjuvants such as fertilizers or pesticides added during the growing process.

These practical problems will need resolution, but not at the basic science level. Moreover, account needs to be taken of the overall energy efficiency of producing the biofuel and its available energy in use [8].

The resultant biofuels will need to operate effectively in the current and future generations of engines in which they will be used. Hence, biofuel composition, its properties, and qualifications need to be considered. This issue is not a basic biofuels production science problem, but it is an integral part of efforts to develop and design next-generation, high-efficiency internal combustion engines [9].

Ultimately "…for biofuels to emerge as a viable alternative to petroleum-based fuels we must develop cost-effective production technologies. The obvious national imperative of the problem has produced a groundswell of research activity in laboratories across the country. The range of high-tech analytical tools, sophisticated software, and powerful computers now available to the scientific community allow researchers to "see" chemical reactions as they unfold. This unprecedented analytical capacity presents exciting opportunities to fine tune biomass conversion reactions and engineer efficient and economical processes for biofuels production. Today, we have both the incentive and the technical means to solve this problem. Through concerted effort and a sustained investment in research we will solve it" [10].

Status of Present and Ultimate Industrial Technology Deployment

The technology for economically converting biomass into widely usable fuels in the second-generation embodiment does not yet have widespread commercial implementation. There are a large number of laboratories in the United States that have capabilities to experimentally demonstrate the chemistry and/or biology to create biofuels. At the pilot and demonstration levels (less than 2 million [MM] gallons per year [gpy] nameplate capacity), there are less than 20 facilities in operation [11]. The commercial level of biofuel production (above 20MM gpy) has no currently operating facilities in the United States; however, there are several in the design and planning stages with planned on-stream operations in 2012 and later.

As described below, the number of technologies that are possible for production of biofuels is large. While these many methods are technically unrelated, the basic science needs underlying each technology are all very similar, as will be discussed in the priority research directions sections.

As optimized processes and economies of scale are attained in later process generations, more widespread distribution of facilities may occur. In particular, if efficiencies can be obtained by collecting and separating municipal solid waste facilities to reclaim primarily cellulosic materials, much broader implementation can be accomplished.

Specific technology areas and their status include the following:

1. There are a large number (more than 50) of laboratories in the United States studying a wide array of methods to convert lignocellulosic biomass to ethanol, and to a lesser extent, butanol. A much smaller number of pilot and demonstration plants exists with capacities from tens of thousands of gpy to approximately 1 million gpy of ethanol. As of

this writing, there are no currently operating commercial facilities in the United States, although several companies have plans for installation and operation over the next one to three years.

2. Gasification, the thermal depolymerization of biomass in the absence of air or oxygen to produce synthesis gas (a mixture of hydrogen and carbon monoxide) has been demonstrated on a small pilot scale, but there is no commercial operation thus far, due to high capital costs and expensive gas clean-up requirements.

3. Thermal pyrolysis — decomposition in the absence of air — is currently practiced without catalysts in commercial operation. Catalytic pyrolysis of biomass is currently still in the research and development stage, with plans to produce a bio-oil that is more stable for extended storage, has higher energy density, and is more amenable to upgrading to fungible fuels. One company is developing catalytic cracking, which is expected to be demonstrated in the near future with commercial availability shortly thereafter.

4. Other technologies have been investigated to produce a liquid product from solid biomass in the laboratory. These include base- or metal-catalyzed depolymerization. To date, these approaches have been tested only in the laboratory and do not appear sufficiently mature for commercialization in the near future.

5. Hydrogen production from biomass and intermediates includes gasification (discussed above), steam reforming of depolymerized intermediates, or aqueous phase reforming of light oxygenates and sugars [12]. Steam reforming has been tested only in the laboratory. Low catalytic activity and fast catalyst deactivation must be resolved prior to commercialization.

6. There is a potentially large supply of biomass that can be obtained by harvesting algae. Numerous studies, including a detailed study by the National Renewable Energy Laboratory in the 1970s, have shown that quantities in the range of 80 tons of algal biomass per acre per year are possible, compared with only 4 tons corn stover per acre per year.

Broad Context for the Priority Research Directions (PRDs)

The science underpinning second-generation biofuel production is immature relative to that of the hydrocarbon-based fuels industry. In order to advance the field, we will need to accurately measure and predict enzyme or catalyst structure/function relationships to quantify process rates and yields. The understanding of physical and chemical transformations that occur during the various stages of processing is necessary to attain the highest possible yield of carbon into fuel. Programs that resolve these fundamental issues are critical for the long term ability to obtain the best lifecycle performance for widespread commercial implementation.

Brief Description of Priority Research Directions

- *Diversity of Biomass and Its Intermediates in Biofuel Processing.* This PRD focuses on developing a fundamental understanding of critical components entering from lignocellulosic feedstocks and during the conversion reactions. Some key components are expected to play important roles in the reaction equilibria and rates, which will ultimately determine the economic viability of the processes. The evolution and fate of these compounds are not understood, and sophisticated in situ measurement techniques are required for a clear mechanistic view of the chemical reactions.

- *Influence of Transport Phenomena on Biomass Conversion.* This PRD seeks to understand the impact of the highly non-ideal fluid environment in biofuel reactors on the transport processes and reaction kinetics. The basic science work involves characterization of heat and mass transport and their impacts on key reaction rates. This understanding is essential to developing high-rate, high-yield, minimal-capital processes. Studies should include surface characterization, including microscopic and spectroscopic methods, to observe enzyme diffusion and reaction rates in real time.

- *Catalyst Discovery, Characterization, and Performance Optimization*. This PRD defines the basic science of catalyst and enzyme structures and how they can be manipulated to optimize performance. This will permit discovery of superior catalysts, enzymes, and process configurations for biomass conversion to vastly improve next-generation technologies, and will lead directly to improved process economics, thereby enabling accelerated introduction of these technologies to the market.

III. PRIORITY RESEARCH DIRECTIONS

A. PRD #1. Diversity of Biomass and Its Intermediates in Biofuel Processing

1. Problem Statement

This PRD focuses on the scientific challenges of converting lignocellulosic biomass from diverse plant matter sources to provide a second-generation biofuel with consistent composition. The challenge is complicated by the need to pretreat the biomass in order to enhance the efficiency of the overall fuel-making process. This pretreatment step is known to increase compositional complexity and is implicated in increasing the variability in second-generation biofuel production. In order to operate a commercially viable biorefinery, a greater understanding of the underlying causes of this variability is required, and methods to prevent or counteract this variability must be instituted. To achieve this, critical components, including pretreatment process intermediates, must be identified and quantified, and the mechanisms by which they impact the desired biofuel-forming reactions must be determined.

2. Executive Summary

The conversion of lignocellulosic biomass to biofuel utilizes materials that are inherently variable and involves a series of reactions that proceed in heterogeneous environments. This is hardly an ideal situation for producing a fuel product that must be highly consistent in properties. Although there is a reasonable understanding of the main reaction pathway to yield biofuel, much less is known of potential biomass feedstock impurities and byproducts formed during pretreatment and their secondary effect on the yield, reaction rate, and product quality of the reaction pathways. In order to reduce the variability caused by these agents, much effort needs to be placed on their identification and quantification, and on the actual mechanistic roles they play in altering the pathways to produce biofuel.

3. Context/Background for PRD #1

An ideal chemical conversion process can be envisioned as starting from a well-characterized, single-ingredient feedstock undergoing conversion in a highly efficient single-step process to provide a well-characterized, single-ingredient product. This is certainly not the case with the conversion of biomass feedstock to second-generation biofuel. Lignocellulosic materials, which are being studied as feedstocks for these biofuels, are inherently more complex than the starch and sugar feedstocks used for first-generation biofuels. Sources for lignocellulosic materials will range from woods, grasses, grains, and other forms of biomass, each having different physical and chemical forms of lignocellulose. Typically, lignocellulosic biomass must be pretreated to improve the efficiency of the later conversion steps to form the product biofuels. However, in a practical sense, the pretreatment process is ill-defined and difficult to control, and the biomass has sometimes been termed "recalcitrant." It is hypothesized that the pretreatment/deconstruction processing steps add to the variability of the in-process material by unintentionally creating poisons for either the catalyst, enzyme, or microorganism that are used to manufacture the biofuel. Numerical simulation on supercomputers is already addressing the molecular-level structure and composition of lignocellulosic biomass [13]. This effort will certainly provide detailed information on factors influencing biomass recalcitrance in the pretreatment step. However, additional information will be needed to understand the complexity of the chemical "broth" that is formed during this process, as it is the composition of this broth that will undergo further chemical manipulations to generate the desired biofuel. As noted in [13], the computer simulation effort will require coordination with experimental process (kinetics) data.

After pretreatment, catalysts (e.g., metal complexes), enzymes, or microorganisms are utilized to assist in the conversion of the biomass to intermediates or directly to the final biofuel product. The rates of conversion and selectivities of the catalysts or enzymes can be adversely impacted by minor components in the feedstock or new agents that are formed during pretreatment. The optimization of the pretreatment process and subsequent processing conditions will be dependent on understanding the sources of variability of the components in the feedstock and later pretreatment intermediates.

Under apparently identical conditions, the processing steps for biofuel do not always proceed identically from batch to batch, resulting in inconsistent product yields and compositions. The observation that pretreatment and hydrolysis of different corn stover lots with essentially "identical chemical" compositions produce different kinetics, yields, and compositions has been described: "Feedstock composition impacts both the total available sugar and the types of sugars to be fermented. We now also understand that compositionally similar feedstocks can differ in their reaction to pretreatment and their resulting enzymatic digestibility, strongly suggesting that it is important to understand the unknown structural factors. Although twenty years of empirical studies have identified leading pretreatment options and a preferred cellulase broth, few studies have examined the structural bases of feedstock variability, pretreatment efficacy, and enzymatic saccharification."[14,15]

Furthermore, it is unknown whether, after the pretreatment of the biomass, a fractionation/separation of the components such as cellulose, hemicellulose, lignin, and a variety of other materials such as lipids, proteins, and microcomponents will improve the overall process or not. This question will need to be answered for each specific process in question, such as torrefaction, liquefaction, flash pyrolysis, gasification, and fermentation.

Numerous options exist for obtaining the various biofuels: for pyrolytic processes the intermediate will be a crude oxygenate that will be catalytically converted into a hydrocarbon mixture, whereas for fermentation or catalytic reforming processes, the pretreatment intermediate will be hydrolyzate, a sugar/starch composition derived from the saccharification of the hemicellulose and cellulose components. The hydrolyzate can be converted into alcohols via fermentation using microorganisms, or to synthetic hydrocarbons by aqueous catalytic reforming. Pyrolysis of biomass to bio-oil has many potential reaction pathways, generating a diversity of compounds, via mechanisms that are not well understood. The lack of understanding of the feedstock composition only complicates the attempt to understand these mechanistic aspects.

4. Industry Need

Since batch-to-batch variability has been observed even when process conditions are stringently maintained, it would appear that the variability is due to undefined components, either in the feedstock biomass or formed during the pretreatment step. Current analytical testing has yet to provide the chemical composition of these components. It is unclear whether these minor components are below the detectable limits for the analytical techniques or whether the current analytical modalities are inappropriate for the task. Once these components are identified and their mechanisms of action understood, remediation measures can be designed to reduce variability to meet biofuel specifications.

In addition to the inherent variability of feedstock, the problem of providing process uniformity is compounded by a lack of understanding of the specific mechanisms that control the conversion processes to biofuels; this is especially true in the case of uncatalyzed pyrolytic processes.

The most likely fuel products will be bioethanol for use in flex-fuel vehicles, and synthetic hydrocarbons as drop-in replacements for petroleum products such as gasoline, diesel, and aviation fuel. For ethanol, the back end of the process will be virtually the same as the current corn starch-to-ethanol first-generation processes. For the synthetic hydrocarbons that will be generated from pyrolytic or catalytic thermolysis processes, there is a greater risk of contaminants remaining in the biofuel (especially in aviation fuels, because of their tight specifications). The aviation fuel market requires a synthetic hydrocarbon drop-in product that will have the most stringent specifications, and therefore, chemical analysis for the overall process will be the most urgent.

5. Scientific Challenges

By far the greatest challenge is the need to obtain useful chemical analyses on the complex mixtures formed after pretreatment. It is likely that the variability seen from batch to batch may be due to concentration changes of components that are at extremely low levels within a complex chemical and multiphase matrix. These components may be found in only certain feedstocks, and in some cases, they may be dependent on the agronomic history of a given feedstock. It is uncertain whether current analytical tools can meet this challenge or whether new modalities will need to be designed. Analysis will need to provide information on quantity and exact structures whether these are from organic, inorganic, and biological materials. Additionally, some of these materials may be stable only under very specific conditions (e.g., enzymes); so analysis may need to be performed in situ and in real time. Having knowledge of the structures of interfering agents and the mechanisms by which they interact with the catalysts or enzymes will allow processes to be designed that will mitigate the impact of these agents without significantly affecting overall yields and cost of the biofuel.

6. Research Directions

Little effort has been applied to understanding the variability of the pretreatment process and the root causes for this variability. The rates of the main hydrolysis/pretreatment reactions and the potential inhibitory role of any component need to be measured to build kinetic models. Measurements should be made in situ to determine whether any product inhibition or catalytic poisons are being formed and at what rates. These concerns must be addressed by (1) identifying the components and the ranges of concentrations that cause variability in the process or impact product quality, (2) using kinetic information to develop a mechanistic understanding the relationship between these components and the observed variability, and (3) designing remedies to ensure robust processing in order to provide consistent biofuel product.

The basic science aspects of this effort will include (1) reducing or eliminating the components that cause variability in the final product through defined agronomic practices, breeding/genetic modification, or chemical means; (2) searching for reaction conditions such as pH, time/temperature, ionic strength, crystallinity, or diffusivity that can reduce their impact; and/or (3) moderating their impacts by modifying the structure of the enzyme, catalyst, or microorganism. Imaging of plant structures at the molecular level and supercomputer modeling of biomass should be useful in supporting the challenges described above.

7. Potential Impact

This PRD is critical to developing increased consistency of the biofuel, which is an absolute requirement for commercialization. Without a robust and consistent process capability, highly undesirable techniques such as blending will be required, which would lead to increased cost and large inventories. Success would open up a new major source of biofuel, complementing or possibly even displacing today's dominant cornstarch-to-ethanol pathway. Its process energy advantages and ability to draw on a much wider array of starting materials would revolutionize the transportation fuel industry.

B. PRD #2. Influence of Transport Phenomena on Biomass Conversion

1. Problem Statement

The conversion of biomass to fluid-phase reaction intermediates and products occurs in highly viscous, non-ideal, and heterogeneous mixtures. The rate-limiting step involves the most expensive components in the process, namely catalysts (including enzymes). Significant improvements are needed to drive more widespread expansion of the biofuels industry. At least two phenomena are not sufficiently understood for optimal process design: transport of catalyst to the substrate (i.e., the reaction site) and surface diffusion. The rates of conversion of biomass are likely to be limited by the rates at which the catalysts and reactants come into contact with each other, which is a bulk fluid phenomenon. Once the catalyst and reactant are in contact, the diffusion of the catalyst on the surface of the reactant is a potential further bottleneck in the degradation of the cellulose. Both aspects of transport in biomass mixtures are unknown, due to the highly viscous, non-Newtonian nature of biomass mixtures, the surface properties of the cellulose, and the constituents on the surface that may inhibit motion of the enzymes. Figure 9-3 shows an illustration of enzyme processes operating both in the bulk solution of the mixtures as well as on the surface of the cellulose. Enzymes (the oval figures) are required to work in the bulk solution and on the surface of the cellulose substrate. The ease with which the enzymes come into contact with the cellulose and the entities in solution such as cellobiose (the dimer of glucose) and glucose will determine the rate at which the cellulose is degraded to the sugar intermediates. Both bulk and surface diffusion must be studied mechanistically and quantitatively to enable the predictive models required for process design and sizing.

2. Executive Summary

A clear understanding of the transport mechanisms and their impacts on reaction rates and selectivities in biomass mixtures — including developed theories and models — is needed to optimize the biomass conversion process. The mixtures in biomass reactors are very viscous and highly non-ideal, and have not been studied on a microscopic scale sufficient to understand the basics of mass transport and their impact on reaction rates. Fundamental measurements leading to mathematical models must be performed in these systems. Imaging and spectroscopy are needed to characterize bulk and surface diffusion under realistic processing conditions.

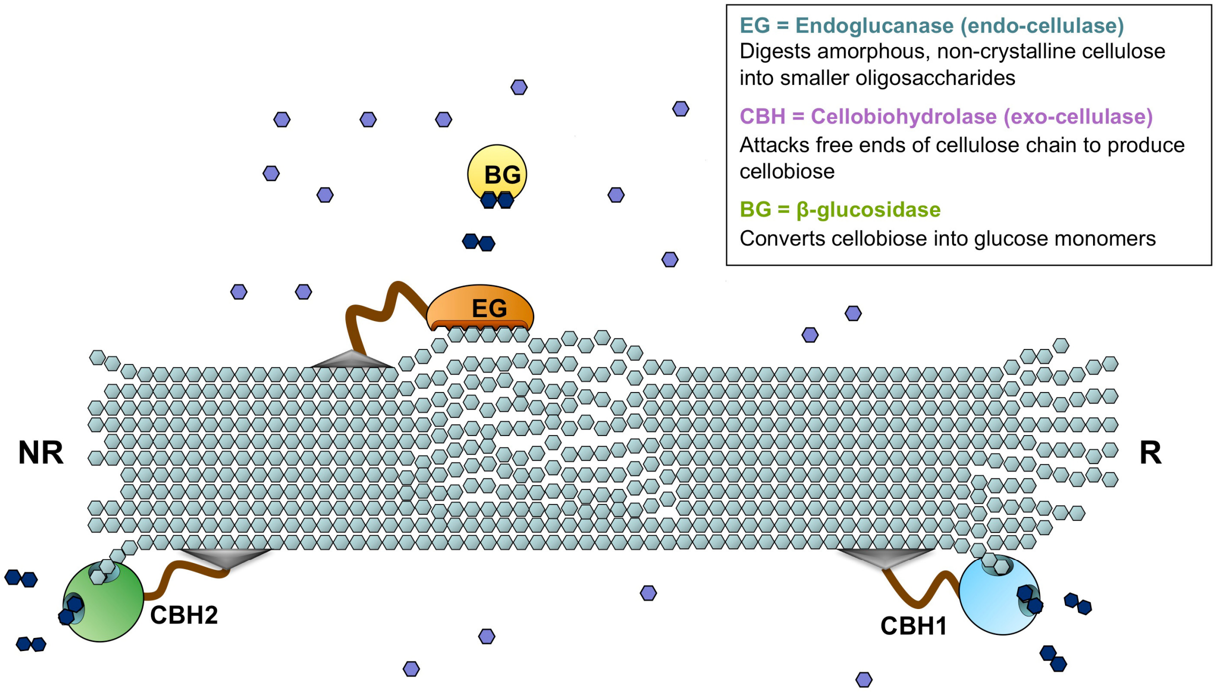

Figure 9-3 Schematic of enzyme actions on cellulose surface and in solution. Source: J. Stege, Verenium Corp. (Copyright Verenium Corporation, 2010)

3. Context/Background for PRD #2

Many different processes will probably be commercialized for converting biomass to biofuels, all with key features in common, namely, that the chemical transformations of the high-molecular-weight feedstocks such as cellulose into fuel-precursors or fuels directly will depend on control of mass and heat transport and process kinetics. This PRD addresses the mass-transport aspect of the process and its impact on overall reaction rates. Understanding this aspect will be instrumental in defining how biofuel reactors are configured and operated as well as what fundamental limitations exist in catalyzed processes using biomass feedstocks.

4. Industry Need

The optimization of capital and variable costs for catalyzed reactions for biofuel depends more strongly on the efficacy of the catalyst than any other factor, and yet catalysis is often the least understood step. Since most biofuels must compete with existing fossil fuels in terms of cost, it is imperative that the biofuels industry develop efficient processes that optimally utilize the biomass. To develop high-rate, high-yield, minimal-capital processes requires detailed understanding of the heat and mass transfer and kinetics of the key reactions. Basic science research is required because the raw materials used in second-generation biofuel processes have not been studied yet from a transport and catalytic rate perspective. The ‘fluids’ that result from the pre-processing steps are complex and have highly non-ideal properties, which are currently believed to limit reaction rate and potentially poison the catalyst, further limiting rate and yield. Obtaining high rate and yield requires enough understanding of the physico-chemical interactions of the catalytic steps so as to allow designing and operating an optimized process. Definitive understanding of the rate-limiting factors will determine plant size and ultimately, process economics. Plants will be similar to petrochemical facilities, as shown in Fig. 9-4.

Figure 9-4 Second-generation cellulosic biofuel demonstration facility. Source: Verenium Corp.

5. Scientific Challenges

The transport of enzymes to the reactants for bio-based processes and of the intermediates to the solid catalysts for catalytic processes must be understood sufficiently to be quantified and useful for reactor design. The medium is likely to be very viscous and non-Newtonian, and as such, mass transfer limitations to overall reactions could be significant. There are no reliable measurements or predictive models that quantify the bulk transport mechanisms and rates in these media. The science should include simulation and model development to represent diffusive transport in highly viscous, non-Newtonian multiphase environments. In addition, surface diffusion, especially in enzymatic systems, must be better understood. As enzymes diffuse on surfaces, the role of surface defects and strongly adsorbed impurities may have a profound impact on the enzymes' ability to function. The events that cause this and the impact on enzymes have not been studied quantitatively, in spite of the fact that the enzymes are the most expensive components in these bioprocesses.

Understanding the behavior of enzymes and catalysts interacting in these complex fluids will become central to cost-effective design of processes and efficient operation of facilities. This is a direct analog to the developments that occurred over the last century in the petroleum refining industry, where the understanding of the fluids and interaction with cracking and reforming catalysts became central to creating the petroleum-based fuels infrastructure we have today. The hydrodynamics, diffusion, and surface interactions are not the same. The morphology, fluid properties, and chemistry of bio-based feedstocks comprise a new field requiring the exploration of the materials and their interactions with the reactive entities.

6. Research Directions

Fundamental measurements should be made in order to develop theories and models of the diffusive transport of large molecules in the complex multiphase biomass mixtures. This should be done so that effects of both mass and heat transport on reaction rates can be predicted.

Specifically, measurements need to be made of the following:

- *Diffusivity of reactants in the bulk mixtures*. Diffusion is hindered by high solids concentration of the substrate and high molecular weight of the enzyme catalyst. The bulk properties and diffusion through them will provide the first barrier to overall reaction rates of converting cellulose to glucose or cellobiose, the dimer of glucose. Investigation of the diffusion could be accomplished with fluorescent or radio-labeled tagging studies to observe the bulk properties as a function of solids loading, pH, ionic strength, temperature, and bulk compounds in solution as described in PRD #1.

- *Diffusion of the enzymes on the surface of the substrate*. Enzymes reacting on a cellulosic substrate must first adsorb to the surface in order to react with the material. When one reaction has occurred, such as the cleavage of a glucose molecule from the cellulose polymer backbone, the enzyme must then remain on the surface of the substrate and diffuse to the next-available reaction site. There, the next monomer may be cleaved from the cellulose. This process must be repeated quickly and millions of times for the cellulose to be reduced to its constituent monomers suitable for conversion into biofuels. Many factors need to be quantified for their impact on the rate of glucose production: cellulose crystallinity, cellulose composition (e.g., portion of 6-carbon, 5-carbon, and lignose molecules), pH, temperature, enzyme type, impurities on the cellulose surface of the cellulose, and whether there are unreactive sites on the cellulose. Such measurements could be made, for example, with fluorescent tagging methods, atomic force microscopy, and conformal laser scanning microscopy.

Such fundamental measurements can be applied to the development of mathematical models that account for both mass transport limitations and fundamental reaction rate equations. Definitive reaction models, including mass transfer, are a requirement for performing quantitative reactor designs, as well as the upstream and downstream process steps for (1) optimization of yield and rate and (2) minimization of capital.

7. Potential Impact

Understanding the interaction of mass transport with reaction kinetics in these systems will enable optimization to faster, lower-cost catalytic conversions of biomass. Obtaining higher yields of the desired products and utilizing all available carbon will enable industrial process development to reduce both capital costs and operating expenses. The primary driver for widespread introduction of biofuels processes on a commercial scale will be highly cost-efficient processes that can compete with today's petrochemical infrastructure. The understanding gained from these programs will be analogous to the evolution of the petrochemical fuel processes that used basic science to understand the key process steps to create efficient conversion technologies. Success in developing such lower-cost processes can vault lignocellulosic biomass into direct and cost-effective competition with petroleum fuels, with huge energy and environmental benefits.

C. PRD #3. Catalyst Discovery, Characterization, and Performance Optimization

1. Problem Statement

There are no commercialized processes today for the conversion of renewable lignocellulosic feedstocks to fuels. Production of ethanol or butanol from cellulose via gasification followed by Fischer-Tropsch or methanol synthesis, and pyrolysis or liquefaction followed by upgrading to drop-in fuels, are in various stages of research and development. Significant improvements in the performance of enzymes and catalysts would substantially improve the process economics and accelerate widespread industrial deployment of these technologies to reduce our dependence on petroleum-based fuels, bringing huge benefits in energy efficiency and greenhouse gas reduction. Biomass conversion improvements could be expected if fundamental catalysis research leads to identification of catalysts optimally suited for these reactions.

2. Executive Summary

Research and development organizations have been working for decades to develop technology for the conversion of biomass to fuels. We propose the development of basic science to understand catalyst and enzyme structures and how they can be manipulated to optimize performance. This basic science will permit discovery of superior catalysts, enzymes, and process configurations for biomass conversion, to vastly improve next-generation technologies. This will lead directly to improved process economics, thereby enabling accelerated introduction of these technologies to the market.

3. Context/Background for PRD #3

The basic science described in this PRD is similar to that in the DOE Basic Research Needs report *Catalysis for Energy* [16]. Figure 9-5 from Huber et al. [17] illustrates some of the fermentative and heterogeneous catalytic routes to fuels from biomass. The fermentation routes of interest for the production of ethanol and butanol are discussed in more detail in the first PRD.

The non-catalytic gasification route to produce synthesis gas, a mixture of carbon monoxide and hydrogen, can be coupled with Fischer-Tropsch synthesis to produce diesel or gasoline. Fischer-Tropsch synthesis for syngas conversion are well established commercial processes. The gasification step has been demonstrated on a small scale, but is not yet commercial. However, gasification has very high capital costs and the gas clean-up is problematic. Widespread use of the gasification approach is unlikely unless capital costs can be reduced.

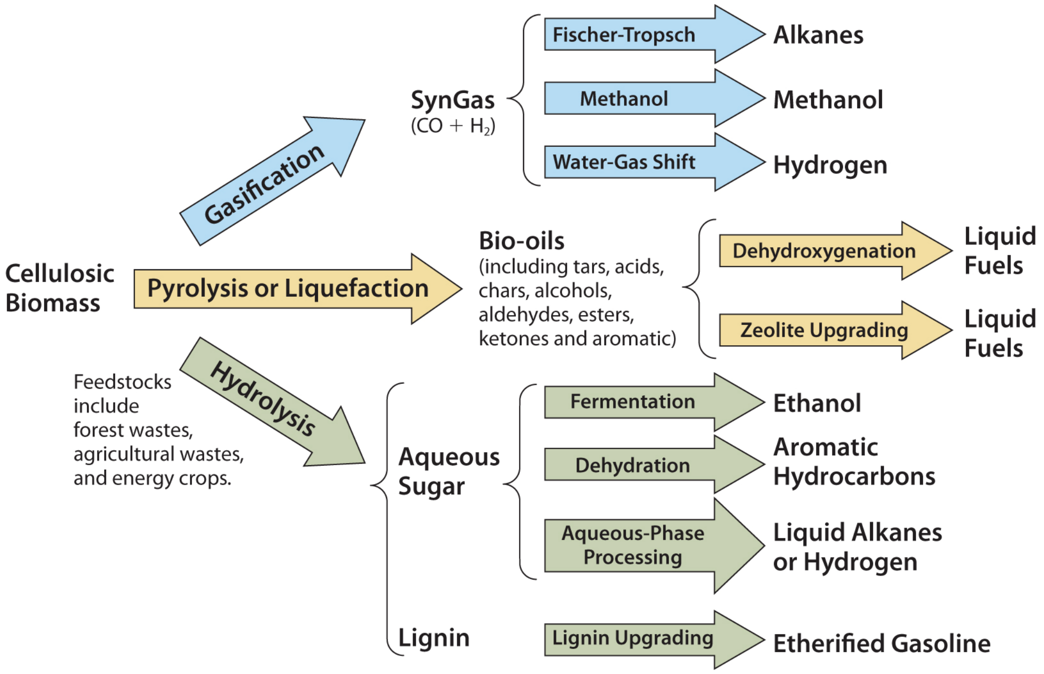

Figure 9-5 Various routes to fuels from biomass. Source: After [17].

Other technologies to depolymerize solid biomass include thermal or catalytic pyrolysis, catalytic liquefaction, and hydrolysis. The products of these processes include acids, aldehydes, phenolics, and sugars. These smaller organic fragments require deoxygenation and further upgrading, for example, by condensation reactions to remove water or hydrodeoxygenation reactions (with hydrogen) to make hydrocarbons.

Enzymatic depolymerization of lignocellulosic materials has been explored for several decades and looks very promising as a commercially viable solution to the challenge of utilizing lignocellulosic biomass for biofuels. Several companies have been successful at engineering the enzymes and optimizing the mixtures of enzymes required to make enzymatic hydrolysis of the cellulose into glucose and cellobiose (the glucose dimer) a practical reality. The many portions of the catalysis work suggested below also apply to these biologically derived systems.

The primary chemistries investigated to date are illustrated in Fig. 9-5. The challenges to research of depolymerization, deoxygenation, and final upgrading include:

- Design of catalytic systems,
- Elucidation of catalyst structure under reaction conditions, and
- Elucidation of the reaction mechanisms and kinetics.

Today, the understanding of the elementary processes involved in these conversion steps and types of catalysts that are best suited to them is still rudimentary in comparison to petroleum processing; therefore, enormous opportunities exist to develop next-generation technologies that will have far better process economics.

The preferred fuel products have significantly low oxygen content compared to the biomass feed. Fermentation eliminates oxygen via elimination of carbon dioxide. In order to preserve carbon, it is often preferable to eliminate oxygen via catalytic hydrodeoxygenation.

Hydrogen for hydrodeoxygenation would have to be produced on site if no refinery is nearby. Currently, hydrogen is produced primarily by steam reforming of methane (which has a large carbon dioxide footprint). Whether mandates to substantially reduce carbon dioxide footprint are issued or not, there will be significant public pressure on all producers to be environmentally conscious. Gasification of biomass or steam reforming of light oxygenated biomass intermediates have been problematic because of high capital cost coupled with fouling of the steam-reforming catalyst. The economical production of hydrogen from biomass or biomass intermediates such as light oxygenates from pyrolysis oil or sugars to reduce carbon dioxide footprint would allow for stand-alone hydrogen production. Alternatively, this technology for hydrogen produced from biomass could be used immediately by refiners, ammonia producers, and other hydrogen users to reduce their carbon dioxide footprints. Aqueous phase reforming (either stand alone or in situ) has been developed as one approach to produce hydrogen, but to date has not been commercialized [12]. As above, the understanding of the elementary processes involved in hydrogen generation and the types of catalysts needed will be required to make substantial catalyst improvements.

4. Industry Need

Efficient enzyme-based catalytic processes for the conversion of biomass to fuels are needed to develop more economical processes. Some of the key chemistries needing improvement include:
(1) generation of hydrogen from biomass or from intermediates derived from biomass,
(2) deoxygenation of biomass or intermediates, (3) condensation of light oxygenates, and
(4) aromatization. Included is the development of catalysts with improved stability under harsh operating conditions in the presence of liquid water or steam, in strongly acidic to basic conditions.

5. Scientific Challenge

To improve catalysts rationally, researchers must understand the impact of catalyst/enzyme composition and structure on performance with biomass processes, as well as mechanisms of catalyst deactivation including coke formation, metal leaching, and support dissolution. Catalysts for these conversions are known, but not nearly well enough, so there is an urgent need to develop next-generation catalysts with significantly improved performance. New technology, such as enzymatic reduction of sugars to alkanes, could be game-changing.

Techniques are available at user facilities, such as in situ spectroscopy and microscopy for model compound studies; these need to be specifically applied to key chemistries. It is important to understand the catalyst-active site and how it changes both structurally and electronically while the chemical reactions are taking place. Additionally, new synthetic techniques will need to be developed to produce these highly active and selective materials not only for laboratory use, but for commercial-scale application.

6. Research Directions

The key basic science contribution is to correlate catalyst/enzyme properties to performance. Through iterative modifications in catalyst composition, confirmed via characterization and correlated to performance, the optimized catalyst can be designed. Researchers have been correlating detailed morphological information with performance. High-Angle Annular Dark-Field Scanning Transmission Electron Microscopy (HAADF-STEM) studies have provided detailed morphological insight regarding supported catalyst nanostructures [18]. The technique allows the catalytically active edges to be imaged even for single-layer metal sulfide structures. The ultimate goal of this work is the design of catalysts using modeling tools.

Finally, improved synthetic techniques such as atomic-level control of catalyst/enzyme structures will need to be developed to synthesize active and highly selective catalysts. It will also become very important to develop novel anchoring or tethering of active metals to supports, in order to minimize leaching in aqueous environments that range from highly acidic to highly basic.

7. Potential Impact

Significant increases in catalyst/enzyme activity, selectivity, and stability will reduce catalyst and recycle requirements, reduce the size of the reactor, simplify the purification train, and ultimately reduce capital and processing costs. This concerted effort will enable fuels from biomass to compete more effectively with current petroleum-based fuels, potentially revolutionizing the transportation fuels industry with major gains in energy efficiency and greenhouse gas reduction.

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Chapter 10: Panel 8 — Energy Efficiency: Buildings, Fuel Cells and Wind Power

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I. EXECUTIVE SUMMARY

Energy is the currency of human prosperity. Historical gains in energy efficiency of generation, conversion, and use over a century have played a major role in meeting the world's energy needs. Going forward, increasing efficiency remains the single lowest-cost and nearest-term opportunity to moderate and meet our nation's demand for energy. Seizing this opportunity requires a surge of innovation that starts with scientific understanding. The largest components of energy use are combustion of fuels for transportation and heating and electricity for lighting, air conditioning, and motors. One focus of this report is on building envelopes in which huge opportunities exist for reducing heating and cooling demands through advanced coatings — glazing for windows and opaque materials for the remaining envelope. Fuel cells that convert chemical fuel to electricity and heat at high efficiency are another ripe opportunity to replace inefficient combustion-based energy production; scientific understanding is essential to developing more cost-effective fuel cells with transformative potential. On the generation side, offshore wind is a reliable and plentiful energy resource for electricity production, provided cost performance can be improved to compete with onshore wind and fossil generation.

II. PANEL REPORT

Role of Energy Efficiency in the National Energy Picture

Increasing energy efficiency has been a predominant factor in the growth of the global and U.S. economy for more than a century. If not for the dramatic decrease in energy intensity (energy required per dollar of economic output) since 1917, the U.S. economy would have required four times today’s energy to produce its current economic output, and the U.S. economy alone would require 85% of today's world production of fossil fuels. As a result of many technological breakthroughs, energy intensity has declined steadily during the last 90 years. For the last 30 years, it has decreased at an average rate of 2.1% per year, twice the average of the previous 50 years, in which the decrease was 1.6% per year (Fig. 2-1). If this rate of energy efficiency improvement could be further increased to 2.5% per year, it would be sufficient to allow the U.S. economy to grow at its projected growth of 2.5% per year until 2030, *without any further increase in energy demand* [1].

But in spite of impressive gains in energy efficiency over a century, the U.S. energy intensity (9113 BTU/$) is still 30% to 50% higher than that of many other industrial nations, such as Japan (4519 BTU/$), Denmark (4845 BTU/$), Germany (7396 BTU/$), and France (7994 BTU/$). In addition, per capita energy use (BTU per person) in these countries is only one-half to three-quarters of that in the United States. The International Energy Agency’s analysis reveals that about half the difference between the U.S. and European per capita energy use is directly attributable to the higher energy efficiency of European economies [2]. The United States can and must do more. The development of new energy-efficient technologies for generation, conversion, and use is the single lowest-cost and the nearest-term opportunity for moderating our nation’s demand for energy.

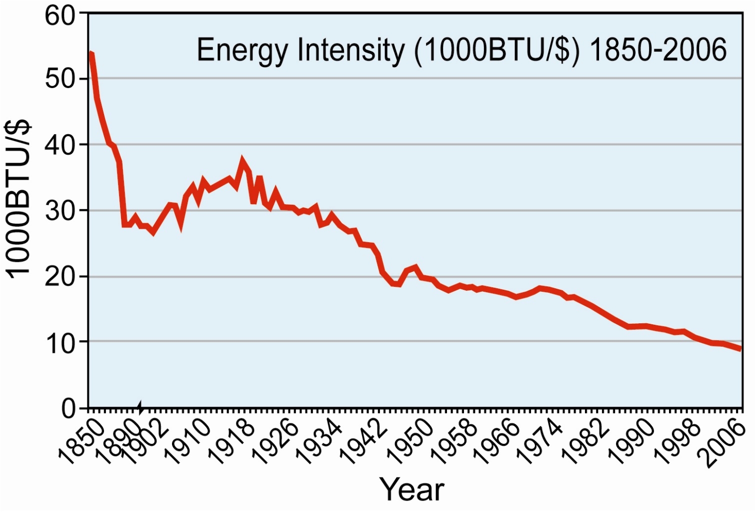

Figure 10-1 U. S. energy intensity (energy use per dollar of gross domestic product [GDP]), 1850–2006. Source: [1].

Current Status and Ultimate Potential

The National Academies Report *America’s Energy Future* concludes that energy savings of 30% by 2030 and 15% by 2020 are cost-effectively achievable by making the U.S. buildings, transportation, and industry sectors more efficient [3]. Meeting such aggressive goals will require increased adoption of existing commercial technologies, including standard high R-value insulation and windows, modern higher-efficiency power plants, and increasing adoption of renewables such as wind power. But that will be not enough. New technologies emerging from discovery of new materials and better scientific understanding of sustainable energy phenomena must be added to the mix. A transformative plan that includes mobilization of basic science to address fundamental challenges is essential to achieve the full impact of efficiency improvement in the shortest timeframe. For example, one can envision an ultimate technology deployment including broad scale overhaul of building envelopes based on new coating technologies to make them near energy-neutral, widespread introduction of new cost-effective fuel cells in stationary and transportation applications to revolutionize efficiency of fuel conversion to electricity, and a major extension of wind power to offshore, doubling this leading renewable source.

Broad Context and Background for the Priority Research Directions (PRDs)

One of the most significant opportunities for increased efficiency comes from use of dynamic optical and thermal coatings in buildings, potentially resulting in a savings of up to 10% in the nation's entire energy use. The scientific challenge is associated with the design and discovery of new materials, and simulation and validation of such coatings.

Another major opportunity for efficiency gains in conversion of chemical fuels to electricity and heat is through the use of fuel cells rather than traditional combustion. Efficiency could reach up to 50% for electricity alone, and up to 80% or more when the waste heat is used for space heating or for additional turbine-based electricity production. Four types of fuel cells are poised for more extensive market penetration: proton exchange membrane, phosphoric acid, molten carbonate, and solid oxide. Each is used in niche market applications, but none has yet achieved its potential for replacing less-efficient combustion-based electricity generation. Cost must be lowered and performance increased to enable broad market penetration. Scientific understanding of the fuel cell conversion processes is essential to developing new materials and chemical processes that will drive widespread adoption.

Efficiency can also be increased through the use of renewable energy, and wind power is one of the most rapidly expanding commercial renewable energy sources, with costs per kilowatt-hour (KWh) approaching that of fossil fuel energy. But this expansion is almost totally terrestrial. Less than 2% of wind power is produced offshore because of higher cost; yet with steadier and stronger offshore wind, this is one of the greatest opportunities for renewable energy expansion. The key to cost-effectiveness of offshore wind power is high reliability offshore turbines with 10 megawatt (MW) and higher ratings, while 6 MW are now the largest demonstrated thus far. The massive gears, generators, and blades required for such ratings using conventional technology are presently showstoppers, and offshore maintenance costs add significantly to electricity cost. New materials for lighter and stronger blades, new understanding of reliability limits of structural components in this demanding environment, predictive modeling based on condition-based monitoring, and new lightweight, high-capacity superconductor generators open promising paths around the obstacles.

Brief Descriptions of the PRDs

PRD #1. Dynamic Optical and Thermal Properties of Building Envelopes

This priority research direction includes work on novel coating materials using nano-materials and novel deposition processes to achieve optical and thermal properties that respond passively or controllably to external conditions for reducing heating and cooling demands by control of light transmissivity and reflectivity or by improved thermal insulation. The impact of such dynamic coatings could be significant on electricity demand and smart grid functionality.

PRD #2. Fuel Cell Materials Understanding and Discovery

The essential materials components of the fuel cell are the cathode and anode, where fuel is oxidized and oxygen is reduced, and the electrolyte that carries cations or anions between the cathode and anode to complete the electrochemical reactions. Each of these components is a sophisticated functional device that requires basic understanding to inspire the improvements that will lower costs and raise performance. The four types of fuel cells closest to widespread deployment — proton exchange membrane, phosphoric acid, molten carbonate, and solid oxide — face different challenges. Materials and chemistry improvements are critical to bringing these four types of fuel cells to commercial viability.

PRD #3. Wind to Electricity — Enabling Material Technologies for Renewable Power

New materials are the focus of this PRD, to enable the larger blades and lighter generators needed for cost-effective offshore wind turbines with high power ratings. Large but power-dense superconductor-based rotating machines, on the scale needed for a direct drive wind generators operating at 11 to 12 revolutions per minute (rpm), have already been demonstrated in a 36.5 MW propulsion motor for the U.S. Navy [4]. To make these systems commercially competitive for wind power, superconductor wire costs — now a major fraction of system cost — need to be reduced. The relevant metric is dollars per kiloAmp-meter ($/kiloAmp-meter); so higher current-carrying capacity can reduce the amount of wire required, and therefore, total system cost. Research into enhancing superconductor-critical current under field and temperature conditions appropriate to this application is needed. A second research direction concerns novel polymeric materials along with fatigue-tolerant, self-healing structures to address the mechanical challenge of larger and lighter blades. Understanding of composite degradation and tools to predict response to damage and fatigue loading is needed. Understanding of aging processes in the metal support structures is a third research area, critical to specifying lifetimes in the aggressive at-sea environment.

Advances in superconductor wires for generator technology also apply to a broader range of rotating machines — utility generators including hydro-generators and a broad array of industrial and transportation motors — which all provide significant efficiency improvements vis-à-vis conventional technology.

While the above three PRDs are considered the highest priorities, many other important areas exist for enhancing energy efficiency. A particularly significant one is in the area of fuel combustion. Given its dominant role in today's economy, combustion is sure to persist for many decades as a major component of our energy system, and natural gas, because of its lower carbon dioxide (CO_2) emission levels than coal, is destined to play an increasing role. Therefore, increasing gas turbine efficiency is a major opportunity. With efficiencies climbing linearly with temperature, operation at up to 1450°Celsius (C) has enabled combined-cycle efficiencies of up to 53% in modern gas-fired combined-cycle power plants [5]. High operating temperature brings the additional environmental benefit of reducing noxious gas emissions like oxides of nitrogen (NO_x).

The key to achieving higher efficiency in gas turbines is developing higher-temperature alloys for the chamber and blades, where the gas combustion occurs, as well as higher-temperature ceramic coatings that protect these alloys. The challenge is similar to developing the alloys and ceramic tiles that protect the space shuttle from the searing temperatures of atmospheric reentry, but the lifetime demands in the combustion environment are far greater — tens of thousands of hours of reliable operation at temperature. A research direction is, therefore, understanding the degradation mechanisms of these alloys and ceramic coatings, which involves new tools for mapping failure evolution in the buried interface between alloy and ceramic, quantitative identification of failure mechanisms, and models that can predict lifetimes of existing and novel materials solutions.

Other opportunities for energy efficiency are treated elsewhere in this report, such as electric power grid efficiency in Chapter 6 (Panel 5) and solid-state lighting in Chapter 7 (Panel 6).

These PRDs overlap some of those developed during the last seven years in the Basic Research Needs (BRN) series of workshops. Generally, the BRN workshops focused on the challenges facing the broad field, while the Science for Energy Technology workshop focused on nearer-term opportunities. The BRN workshop on the hydrogen economy covered many of the ideas in presented here, with an emphasis on proton exchange membrane and solid oxide fuel cells. The BRN report on superconductivity emphasized discovery and fundamental understanding of new materials, mechanisms, and critical currents of superconductivity, while this report focuses specifically on superconductor wind turbine technology as an immediate opportunity to expand our energy supply without carbon emissions. No BRN report addressed the topic of building envelopes, a particularly important area given its huge potential impact.

III. PRIORITY RESEARCH DIRECTIONS

A. PRD #1. Technologies and Dynamic Optical and Thermal Properties of Building Envelopes

1. Problem Statement

Buildings consume 40% of the total energy used in the United States and 72% of the nation's electrical output [6]. It is economically possible to reach cost-effective savings of 30 to 50% of the energy used in buildings and technically possible to extend savings to 70%. Although the technology for achieving such savings has been demonstrated, much of it is not yet sufficiently cost-effective to penetrate widely. Achieving the lower costs and higher performance required for widespread commercial adoption will require basic understanding and control of the materials and chemistry of materials to dynamically control light transmissivity and reflectivity and thermal insulation for energy efficient building envelopes.

2. Executive Summary

Increasing building efficiency is perhaps the single largest area of potential energy savings in our economy. There are rich opportunities for a new generation of passive and actively controllable coatings for both window and opaque building surfaces, to dynamically adjust optical and thermal properties with increasingly cost-effective and durable materials. The scientific challenge is in designing and fabricating new materials structures, often composed of complex nano- or micro-scale multilayers, which meet demanding application requirements. The research directions focus on novel nano-materials as well as new coating techniques based on solution chemistry and deposition.

3. Context and Background for PRD #1

The U.S. buildings sector comprises 113 million homes and 2 billion square feet of commercial space; it uses 73% of electricity and 40% of all energy consumed [6]. It provides one of the largest opportunities for reducing the nation's energy consumption with low cost and high return through development and deployment of improved energy efficiency [7]. By 2030, a combination of currently available and emerging building efficiency technologies could lower building energy use by 25% to 30% [8]. The Energy Efficient Buildings study sponsored by 14 multinational companies in partnership with the World Business Council for Sustainable Development using data from the economies of Brazil, China, European Union (EU), India, Japan, and the United States shows that an annual investment of $150 billion (B) in energy efficiency investments in buildings would cut the global carbon footprint by 40% with a five-year discounted payback [9].

The three largest energy-consuming end uses in the buildings sector are heating, cooling, and lighting, constituting more than half of all energy used in buildings. Opportunities for increasing lighting efficiency are great and are covered in Chapter 5 by Panel 6; here, we focus on new technologies for building envelopes, including windows, walls, and roofs.

4. Industry Need

Five critical performance needs would improve building efficiency and potentially convert the building envelope to a net supplier of energy [7,10]. These include the following

- Dynamic active control of solar-optical properties of window glazing that would modulate solar gain and daylight, control glare and provide thermal comfort (see Figs. 9-2 and 9-3) [11,12].
- Dynamic passive response of solar-optical properties of the opaque envelope of buildings (roofs and walls) that would minimize peak cooling impacts by controlling reflectivity [7,13,14,15].
- Controllable thermal properties of building envelope elements (thermal conductivity, radiation absorbance, thermal storage) that would allow admitting, rejecting, or storing heat to optimize building performance [7,16].
- Passive and active optical properties for windows that would allow spectral diffusion and redirection of incident sunlight [17,18].
- Improved performance/cost ratios for all materials solutions, along with durability enhancement and broad dynamic ranges that accommodate new and retrofit applications [7].

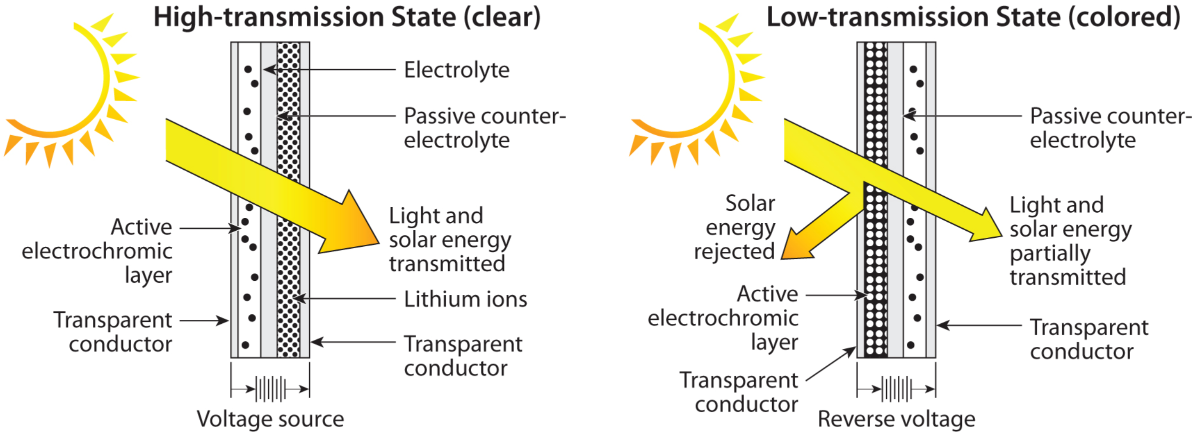

Figure 10-2 Schematic of a typical electrochromic window in clear (left) and colored/opaque (right). Source: "A Design Guide for Early-market Electrochromic Windows," prepared by Lawrence Berkeley National Laboratory (LBNL), May 2006 (CEC-500-2006-AT16).

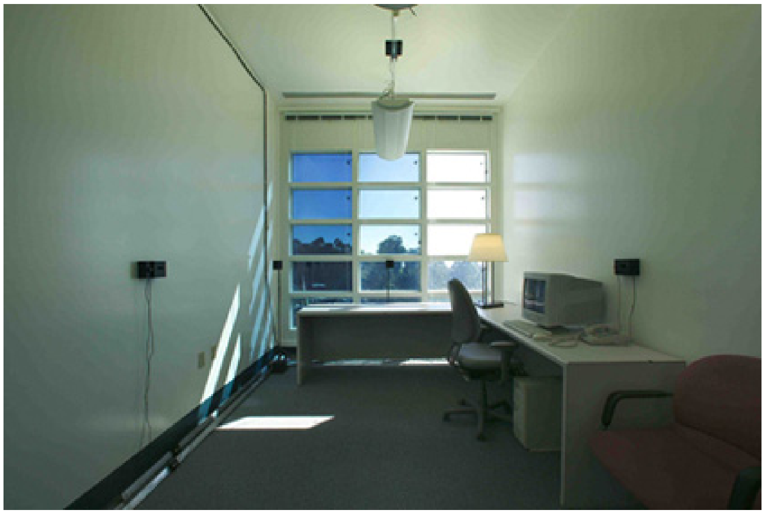

Figure 10-3 Switchable electrochromic windows provide variable solar, daylight, and glare control, shown at the LBNL Windows testbed facility. Source: http://lowenergyfacades.lbl.gov/technologies.html.

5. Scientific Challenges

Five scientific challenges emerge from these industry needs; these are detailed below.

Window, wall, and roof coatings. Actively switchable optical coatings on glass, polymers, and various opaque surfaces require dramatically improved dynamic range, durability, switching speed, and appearance. The largest energy benefits accrue in window applications, but switchable optical properties have value for roofs and walls in many climates as well. Many active coatings are multilayer structures where control of layer-by-layer composition, interfaces, stoichiometry, and microstructure dictate performance [12,18]. Most existing work has focused on electrochromic materials (inorganic and organic) although other optical switch mechanisms are known and could be further explored (see Figs. 9-2 and 9-3) [18]. Most active devices employ transparent conductors, but new materials are needed with very high optical transmittance and very low sheet resistance. Switching across a transmittance range of 60% to less than 1%, in seconds rather than minutes, and lifetimes in excess of 50,000 cycles, is desirable.

Passively triggered dynamic materials. While actively controlled coatings normally have the greatest performance benefits, passively triggered optical coatings are also promising [18] including photochromic and thermochromic materials [12,18]. Although the device structure is normally simpler, and therefore, potentially cheaper to fabricate than active coatings (e.g., no transparent conducting layers), the challenges of switching range, switching speed, spectral response, and lifetime remain.

High-performance opaque envelope materials. Order-of-magnitude improvements are needed in conductivity, heat capacity, and moisture permeability over conventional opaque envelope materials. Additional benefits would accrue if the properties could be dynamically altered, i.e., turned “on” or “off” as needed. In addition to reducing energy use, the dynamic management of peak cooling loads is critical to managing electric load in a future smart grid. The ability to add thermal capacity (cool storage in summer and heat storage in winter) to buildings requires a new generation of intrinsic or encapsulated materials with high thermal capacity, high (or variable) conductivity to add or extract heat, low toxicity and flammability, and cost [13,15].

High-rate, low-cost, large-area manufacturing. Large-area coating deposition has made enormous strides, but remains an art even after decades of applied R&D [12]. Plasma processes in physical vapor deposition and chemical processes underlying chemical vapor deposition and plasma-enhanced chemical vapor deposition are not well understood; breakthroughs here could lead to vastly improved coating quality as well as productivity enhancements that reduce multilayer coating product cost. It is not uncommon for energy control coatings to have in excess of 20 layers, with some only nanometers thick.

Computational tools for materials-by-design. Well-developed computational tools for multilayer coatings exist, although appropriate optical constants for all component layer materials are often not well known, even if their bulk properties are known. A greater challenge is to develop accurate new tools predicting optical and thermal properties and performance from fundamental atomic properties and to extend these tools to realistic models of the chemical processes, kinetics, and thermodynamics of the actual coating deposition production environment so that materials can be “designed” to meet specific functional needs.

6. Research Directions

Window glazing. Materials research and development (R&D) should focus on new materials by design and synthesis to replace electrochromic tungsten and associated materials systems. New device structures that work by reflection, as well as absorption, and solutions that provide spectral control and continuous optical control across their dynamic ranges are needed. Existing multilayer materials designs need to be improved with layer substitution, new materials, and new deposition parameters to improve optical range, switching speed, and lifetime [12]. New materials include vanadium dioxide (VO_2), tungsten trioxide (WO_3) and nickel oxide (NiO) [12,18]. Nanotechnology-based solutions should be explored in conjunction with or in place of conventional multilayer thin film processes.

High-performance opaque envelope materials. New thick film/thin film manufacturing approaches should optimize physical and chemical vapor deposition with ion assist. Improved low-temperature physical and chemical vapor deposition using ion-assisted or plasma-assisted processes suitable for roll coating and deposition on polymeric substrates would provide new capabilities. One of the most promising new directions in basic science over the last decade has been to understand and control the size-dependent optical properties of nanomaterials. This understanding can now be leveraged and applied to thick film solution-based deposition with nano-inclusions and self-assembled nanostructures. Entirely new coating processes not based on physical or chemical vapor deposition, such as liquid phase or spray deposition, that can be scaled to commercial processes, are needed. Biomimetic approaches offer a further set of functional designs and new approaches to fabrication of high-performance optical and thermal control structures.

Variable and reversible heat transfer rates. Explore mechanisms and materials that allow controllable heat transfer rates, reversible heat flows, and high heat capacity/storage/transfer [10].

7. Potential Impact

Innovations in the thermal and optical properties of coating materials could impact heating, cooling, and lighting in virtually every building, and produce energy savings potentially approaching 10% of all U.S. energy use. On a hot summer afternoon, almost half of the utility peak load is driven by cooling and lighting use in buildings, both of which could be reduced with the envelope technologies identified here. Research results could be quickly translated into market savings because the industrial infrastructure for many types of high-volume, low-cost physical and chemical vapor deposition coatings exists today. The controllable dynamic coatings envisioned here could also have a significant impact on smart grid operation, as smart windows help to actively manage energy use.

B. PRD #2. Fuel Cell Materials Understanding and Discovery

1. Problem Statement

Fuel cells offer high conversion efficiency of chemical fuel to electricity and heat, up to 50% for electricity and over 80% if the waste heat is used for combined heat and power. However, commercialization in stationary electricity generation and transportation has been limited by performance, durability, and/or cost of the cathodes, anodes, and electrolytes used in their design.

2. Executive Summary

Fuel cells are potentially important elements of a more efficient national energy system, including both stationary and transportation applications. However, materials discovery, development, and implementation are needed to raise performance and lower cost of these technologies to achieve widespread commercial use. Four types of fuel cells, differentiated by their electrolyte and the temperature at which they operate, have broad commercial potential. Proton Exchange Membrane Fuel Cells (PEMFCs, 80°Celsius [C]) and Phosphoric Acid Fuel Cells (PAFCs, 200°C) are constrained by cathode stability and cost; both of these systems currently require platinum-based catalysts. Molten Carbonate Fuel Cells (MCFCs, 650°C) and Solid Oxide Fuel Cells (SOFCs, 600–1000°C) are attractive for stationary power use, but are subject to materials degradation and failure due to high-temperature cycling of the cathode, electrolyte, and interconnects between cells in the stack. Basic research focused on the commercialization-limiting materials problems can enable these fuel cell technologies to play a key role in our nation’s energy system.

3. Context and Background for PRD #2

Fuel cells, shown schematically in Fig. 10-4, are devices that convert chemicals into electrical energy and heat. This is achieved by oxidation and reduction reactions in anode and cathode compartments separated by an ion conducting membrane. Electrons do work as they are transferred between electrodes through an external circuit (shown as *Load* in Fig. 10-4). Cations or anions travel through an ion-conducting electrolyte to meet electrons, oxidize the fuel, and reduce the oxidant, producing water and heat. The four kinds of fuel cells described here rely on the hydrogen ion or hydron (H^+) as the cation or the oxygen ion (O^{2-}) as the anion. A fuel cell can be thought of as a continuous battery — as long as reactants are fed and products removed, it will produce electricity. Reviews of the operation and technology outlook for fuel cells are available [19,20,21].

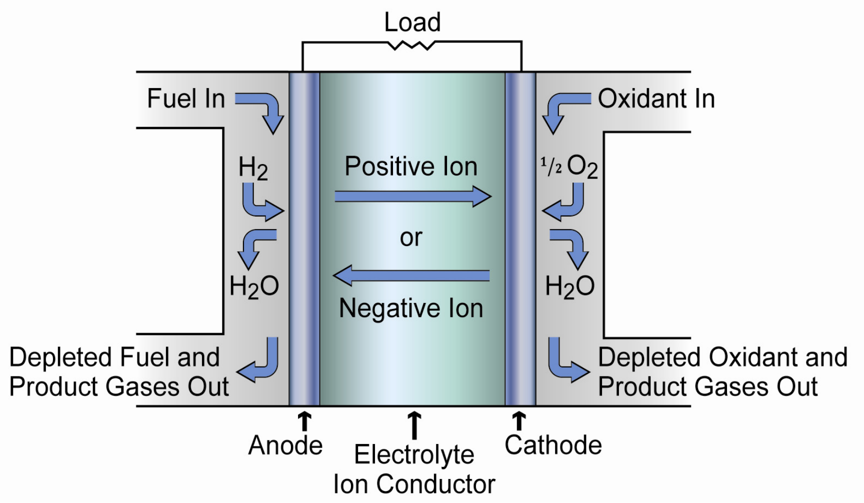

Figure 10-4 General schematic of a single fuel cell. Source: [19].

Four types of fuel cells, whose properties are summarized in Table 10-1, have reached a maturity allowing initial market penetration.

Fuel Cells for Stationary Applications. High-temperature fuel cell technologies such as MCFCs (650°C) and SOFCs (600–1000°C) are most attractive for industrial, commercial, and residential building sectors because of their ability to convert hydrocarbons directly into electricity without an external hydrocarbon-to-hydrogen reformer [22,23,24]. Additionally, their high quality (high-temperature) waste heat can produce electricity by generating steam to run a turbine, resulting in overall chemical-to-electricity conversion efficiencies greater than 80%.

Table 10-1 Key Features of Four Fuel Cell Types with Greatest Application Potential

	PEMFC	**PAFC**	**MCFC**	**SOFC**
Electrolyte	Hydrated proton exchange membrane	Immobilized Phosphoric Acid in SiC	Immobilized Liq. Molten Carbonate in $LiAlO_2$	Perovskites (Ceramics)
Electrodes	Carbon	Carbon	Nickel and Nickel Oxide	Perovskite and perovskite/metal cermet
Catalyst	Platinum	Platinum	Nickel and Nickel Oxide	Perovskite and perovskite/metal cermet
Interconnect	Carbon or Metal	Graphite	Stainless Steel or Nickel	Nickel, Ceramic, or Steel
Temperature	40–80°C	200°C	650°C	600–1000°C
Charge Carrier	H+	H+	CO_3^{2-}	O^{2-}
External Reformer	Yes	Yes	No for some fuels	No for some fuels
Largest Impact Application	~100 kW[a] for Transportation	~200–400 kW for Distributed Stationary	250–2000kW for Stationary Combined Heat and Power	1–1000kW for Stationary Combined Heat and Power
Maturity	Pre-Commercial Prototypes	Commercialized at Low Volume	Commercialized at Low Volume	Commercialized at Low Volume

[a] kW = kilowatt

Source: adapted from Table 1-1 in [19].

Lower-temperature fuel cells can be employed in stationary applications if an isolated reformer is located upstream to produce hydrogen. PAFCs (200°C) can achieve efficiencies of 60% to 80% when integrated with a building in which the waste heat can be used for space heating. United Technologies sells up to 50 units per year (approaching a cumulative 300) in the 200 to 400 kilowatt (kW) range. The PEMFC (80°C) has been developed for stationary applications using reformed natural gas, but the relatively low temperature waste heat limits efficiencies to no more than 50%, and consequently, development for this application has been slowing worldwide.

Fuel Cells for Automotive Applications. The PEMFC addresses automotive applications, due to its ability to start up quickly from a frozen state and to respond to the transient operation of the automotive drive cycle. These fuel cells achieve hydrogen-tank-to-wheel efficiencies of 50% to 60% in midsize passenger cars, compared to less than 25% for gasoline-tank-to-wheel efficiencies in internal combustion applications [25]. Their efficiency advantage is offset by the need to supply relatively pure hydrogen by, for example, water electrolysis or reforming natural gas. Viability depends on the future cost of energy, infrastructure, and vehicles, as well as the value society places on energy use and associated emissions.

4. Industry Need

The primary industry need is to lower fuel cell cost and improve performance so as to enhance commercial viability compared to fossil fuel-based energy generation. Each fuel cell type has special needs:

PEMFCs. The two most serious materials challenges are (1) promoting the oxygen reduction reaction at the cathode and (2) the proton exchange membrane, typically Nafion®. The oxygen reduction reaction is inherently sluggish and requires catalysts, typically platinum. Cathode technology available today allows less than 30 grams (gm) of platinum (Pt) per vehicle with 5500 hours of life, but large market penetration requires less than 5 to 10 gm of Pt per vehicle. At $1200 per troy ounce (oz) of Pt, this translates to $200 to $400 per vehicle, at the high end of the cost of the Pt, palladium (Pd), and rhodium (Rh) in typical catalytic convertors. Even at this level, high market penetration could require large increases in Pt production. Nafion operates effectively as a proton exchange membrane only in the presence of water, limiting operating temperatures to below the boiling point of water. Higher-temperature operation would raise the oxygen reduction reaction rate and reduce the need for Pt catalysts.

PAFCs. The capital cost target for stationary electric power and heat generation by PAFCs is less demanding than for automotive PEMFCs, <$1000 per kW for PAFCs compared to <$100/kW for automotive PEMFCs. Stack life is the critical issue, the state-of-the-art being about 40,000 hours of operation, or about five years, and to increase market penetration, it needs to be extended by a factor of two. The cathode is a key life-limiting component, and solutions are needed to increase or retain cathode chemical activity to meet the durability requirement.

MCFCs. The severe oxidizing conditions present at the cathode limit the number of metals that can be used as electrocatalysts. Lithiated nickel oxide cathodes slowly dissolve in molten carbonate and limit cell lifetime. Nickel oxide cathodes react with carbon dioxide in the molten carbonate electrolyte to produce nickel ion (Ni^{2+}) that diffuses through the electrolyte, is reduced to metallic nickel and deposits on the anode. Continued deposition of nickel (Ni) in the anode region eventually leads to a short circuit between the anode and cathode. Before shorting, however, cathode dissolution removes active material, decreases the active surface area available for the oxygen reduction reaction, and degrades fuel cell performance.

SOFCs. The high operating temperature of SOFCs, 800° to 1000°C, poses multiple challenges to their performance and cost [26]. High temperatures lead to high thermal stress due to thermal expansion, ultimately producing cracking and failure. Long warm-up times mitigate cracking due to thermal stress, but significantly lower commercial viability and raise operating cost. Sealing the multilayer components of a fuel cell is difficult at high temperature, as the differential thermal expansion of the sealant and construction materials is severe. Surface areas also decline at high temperature, as coarsening and sintering grow the particulate size.

The high operating temperature also affects the interconnect materials and bipolar plate connecting the cells in a stack, which must survive reducing and oxidizing atmospheres while maintaining high electrical conductivity and negligible ionic conductivity. Metals and alloys do not fulfill these conditions; thus, interconnect materials are typically ceramics based on the perovskite system lanthanum chromite ($LaCrO_3$). Lowering the operation temperature would allow metals and alloys to be used for interconnects, significantly raising performance and lowering cost. The ohmic losses in a metallic bipolar plate are small, and the excellent heat conduction allows the heat generated at the air electrode to be naturally transported to the fuel electrode to promote the endothermic reforming reaction, eliminating the need for cooling fluid. In short, the fundamental path to raising performance and lowering cost of solid oxide fuel cells is lowering the operating temperature from 800°–1000°C to 600°–800°C.

5. Scientific Challenges

PEMFCs. The sluggish kinetics of the oxygen reduction at the cathode reaction are poorly understood, due to the complex sequence of steps requiring dissociation of oxygen molecules, the formation of one or more intermediate species, and the final synthesis of the water molecule. Neither the active sites nor intermediate states (which may vary with conditions) are definitively known, even for standard platinum catalysts. The relationship between nanoscale material structure and kinetic behavior in PEMFC environments is an important and fertile area for scientific research.

PAFCs. The life-limiting mechanisms of degradation in phosphoric acid fuel cells are associated with carbon-supported Pt catalyst poisoning, coarsening, and dissolution. Phosphoric acid adsorbs quite strongly on the surface of the Pt catalyst, reducing the oxygen reduction reaction kinetics. Fundamental understanding of this adsorption and its impact on the oxygen reduction reaction is needed to guide discovery of materials and phenomena that mitigate or prevent Pt catalyst poisoning.

MCFCs. Doubling lifetime requires replacing nickel oxide (NiO) cathodes with new cathode materials that have (1) low electronic conductivity, (2) general physical stability in both oxidant and molten carbonate conditions, (3) low solubility and no tendency to precipitate upon dissolution, and (4) high density pore structure with good wettability characteristics.

SOFCs. Lowering SOFC operating temperature to 600° to 800°C creates significant materials and chemistry challenges. The ionic conductivity of the oxide electrolyte drops strongly with temperature, limiting reaction rate and power density. Lower temperatures inhibit catalytic activity of the hydrocarbon-to-hydrogen reforming process, requiring new anodes that catalyze the reforming reaction at intermediate temperatures. At the cathode, lower temperature lowers oxygen reduction reaction kinetics. The reaction takes place at the three-phase boundary between oxygen gas, electrode, and electrolyte, whose effective active region can be increased by using mixed-ion electron conductors that absorb neutral oxygen as cathodes. The surface chemical exchange rate and oxygen solid-state diffusion rate at the cathode are key bottlenecks in promoting the oxygen reduction reaction. Replacing ceramics in the interconnect materials with metals and alloys lowers cost but induces oxide scale plating on the interconnect's cathode side, introducing a high electrical resistivity. Metal interconnects also allow transport of gaseous chromium compounds such as chromium trioxide (CrO_3), dihydroxy(dioxo)chromium ($CrO_2(OH)_2$) and chromium hydroxide ($Cr(OH)_3$) into the porous electrodes and subsequent formation of manganese chromite ($MnCr_2O_4$) or nickel chromite ($NiCr_2O_4$), lowering electrode reaction rates [27].

6. Research Directions

PEMFCs. To achieve automotive loading targets, platinum catalysts will need to be replaced with platinum alloys, platinum-shell/affordable-core materials, or preferentially faced nanostructures such as platinum-nickel alloy (Pt_3Ni (111)) [28]. Further research is needed to guide integration of these active materials into practical electrodes without adding significant mass transport losses. Good progress has also been made with Pt-free catalysts; the milestone of meeting the initial activity of Pt-based catalysts has recently been met, however, only at very low current densities and with poor durability [29]. New in situ tools are critical to identifying the active sites of oxygen reduction reaction catalysis, such as environmental transmission electron microscopy (TEM) and electrochemical cells for X-ray spectroscopy. Computational materials and chemistry promise significant new predictive ability in modeling and screening candidate materials for catalysts [30]. Materials synthesis, discovery, and characterization are key activities for bringing proton exchange membrane fuel cells to competitive viability.

PAFCs. Proton conducting materials operating in the 170° to 190°C range that do not adsorb on Pt are needed to replace the phosphoric acid electrolyte, while retaining low-vapor-pressure and thermal stability. Experiments are needed to isolate and understand the mechanisms of Pt dissolution and coarsening as a function of temperature and potential.

MCFCs. The search for cathode materials with slower dissolution in the molten electrolyte takes three directions: coating the cathode with an anti-corrosive protective layer, doping nickel oxide to slow down dissolution, and trying new materials such as lithium cobalt spinel ($LiCoO_2$) for its low reactivity with molten carbonates. The dissolution rate depends on carbonate solution pH, and thus, on other cations in the electrolyte mix, creating a rich multiparameter phase space to search for promising trends. The uncoated conventional NiO cathode can be doped with iron (Fe), magnesium (Mg), and other cations to adjust pH and slow the corrosive reaction. New cathode materials such as lithiated transition metal oxides are promising candidates [31].

SOFCs. Lower operating temperatures, in the 600° to 800°C range require, electrolytes with higher ionic conductivity. One promising solution is to reduce electrolyte layer thickness, which shifts the rate-limiting step from bulk diffusion to surface exchange. Thin electrolytes, however, promote pinholes and cracks, causing cross-mixing of electrolyte gases and lowering cell performance. Higher ionic conductivities can be achieved with new electrolytes, with structures in the fluorite, oxygen-deficient perovskite, pyrochlore, apatite, or scheelite families [32]. To understand ionic conduction in these materials, in situ experimental studies and computational models are needed to analyze and enhance conduction pathways [33].

Lower operating temperatures reduce anode catalytic activity for direct use of hydrocarbon fuels such as natural gas. Novel anode materials are needed, such as $Ni/Sm_{0.15}Ce_{0.85}O_{2-\delta}$, $Ir/Ce_{0.9}Gd_{0.1}O_{2-x}$, trimetal $Fe_xCo_{0.5-x}Ni_{0.5}/Sm_{0.2}Ce_{0.8}O_{1.9}$, $Ni/Ca(Fe)TiO_3$ and Ru/YSZ [34,35]. Cathodes suitable for operation at lower temperature must have higher catalytic activity for the oxygen reduction reaction while maintaining high surface area of the three-phase gas/electrolyte/electrode boundary. Layered mixed ionic electronic conductors such as La_2NiO_{4+x} and $GdBaCo_2O_{5+x}$ promise to fulfill this condition, their oxygen diffusion anisotropy and cation ordering enhance oxygen transport, low activation energies, and high surface exchange, making them appealing for lower temperature operation [36].

7. Potential Impact

PEMFCs. Low-Pt technology would remove the largest and highest uncertainty cost element of the fuel cell vehicle, enabling automotive commercialization. Light-duty vehicles consume approximately 20% of nation's energy and produce approximately 20% of greenhouse gas emissions, and they consume more than 40% of the nation's petroleum, 60% of which is imported. Thus, the potential impact of fuel cell vehicle technology is very large, provided a hydrogen production and distribution infrastructure to support high market penetration can be implemented. Initial penetration will be in smaller market applications such as forklifts and back-up power.

PAFCs. Improvement of cathode durability would lead to increased stack life, enabling substantially increased technology penetration due to lower annual capital cost. This technology is ideally suited for building power and heat, since the 200°C waste heat is sufficient for building heating. Insertion of the technology could occur immediately into the existing product line, with significant market impact.

MCFCs. The potential market for molten carbonate fuel cell power plants in the 200 to 2000kW range operating directly on hydrocarbon fuel is large, and includes hospitals, schools, universities, hotels, and other commercial and industrial applications. Compared to existing fossil fuel technology, such power plants offer higher fuel efficiency, significantly lower emissions, quieter operation, flexible siting and permitting requirements, and scalability. Using the high-quality exhaust heat for cogeneration raises total efficiency above 80% and can provide high-pressure steam, district heating, and air conditioning. Waste heat can also be used to drive a gas turbine for further electricity production. Because hydrogen is generated within the fuel cell module from readily available fuels such as natural gas and wastewater treatment gas, these fuel cells are viable today without a hydrogen infrastructure.

SOFCs. Raising SOFC performance and lowering cost enables a host of applications. Large–scale, high-efficiency, multi-megawatt (MW) power generation is a longstanding target, where continuous operation at 800° to 1000°C minimizes the challenges of materials failure due to thermal cycling. Temperatures of 600° to 800°C enable smaller-scale units, down to 1 kW, for residential and commercial combined heat and power [9]. Auxiliary power units for transportation could provide electricity for heating, refrigeration, and accessories in large trucks. SOFC operating temperature is high enough to drive turbines for electricity production, potentially bringing total chemical fuel-to-electricity efficiency above 80%.

C. PRD #3. Enabling Material Technologies for Next-Generation Wind Power

1. Problem Statement

Offshore wind power is a huge renewable energy resource, but it requires next-generation technology to be commercially competitive. Materials research is needed to dramatically increase the performance of superconductor wires for high capacity (10-MW class) wind generators, to develop stronger and lighter materials for the larger blades required, and to understand mechanisms of degradation and failure in the aggressive offshore wind environment.

2. Executive Summary

Through basic materials research, more efficient and cost-effective technology can be developed to address the tremendous opportunity of increased renewable energy through offshore wind power. To become commercially cost-competitive, offshore wind power requires a new generation of technology based on high-capacity, lightweight, superconducting generators, and larger, lightweight, mechanically stable turbine blades. Fundamental research includes fatigue-tolerant self-healing composite structures for blades, higher current capacity of superconductor wires, and understanding degradation and failure mechanisms based on accelerated materials testing.

3. Context and Background for PRD #3

The U.S. Department of Energy (DOE) and others project that 20% of the nation's power needs can be met by wind by the year 2030 [37]. Many challenges must be overcome to meet this goal, including developing new wind turbine technologies and new grid system capabilities to transmit renewable power to users. Advanced materials provide the needed breakthroughs in equipment efficiency for offshore wind power to make a major contribution to the goal.

4. Industry Need

Optimizing wind turbine system cost has led to larger and larger wind turbines. This is of particular importance to bring offshore wind power into viable commercial competition with fossil energy. Power ratings in the range of 10 MW and higher are needed. Such wind turbines will require towers over 160 meters tall with blades as much as 90 meters in length; this will require novel high-strength materials for the blades and better understanding of the strength and fatigue of structural materials for the tower and drive train. Avoiding gears, which cause significant maintenance and reliability problems, is also highly desirable. Superconductor direct-drive generator technology not only avoids gears, but also dramatically reduces size and weight.

5. Scientific Challenges

The scale-up of wind turbines will require 10-MW generators directly driven at 11 to 12 rpm. A conventional generator at this rating may weigh well over 300 metric tons [38]. This weight must be carried by the tower, increasing the costs of the structure and overall system. Using lossless superconductors in the field winding of these generators can reduce the top weight by a factor of two, as well as improve efficiency. Thus, the scale-up of wind power requires higher-performance, cost-effective superconductor materials.

The scientific challenge for superconductor materials emerges from the cost-performance metric of dollars per kiloAmp-meter ($/kAmp-meter). At present levels of performance, hundreds of thousands of meters of wire are required for the field windings of a multipole 10 MW direct-drive superconductor generator, and at present prices, this is a dominant component of total cost. Increasing the superconductor-critical current by a factor of two would decrease this cost component by a factor of two. The superconductor windings of these machines typically operate in magnetic fields of several Tesla in a conduction-cooled environment in the 30 to 40 Kelvin (K) range, though higher operating temperatures are always desirable for improved efficiency and reduced refrigeration requirements. The mechanisms controlling critical current in this operational range need to be elucidated to design new materials synthesis routes for higher critical current performance.

This scale-up to 10-MW power rating also requires light- and fatigue-tolerant materials for the long length wind turbine blades. The cost of unscheduled maintenance will have a catastrophic impact on the cost of offshore wind power. An unplanned outage offshore can take a turbine offline for six months, as many sites are not serviceable in winter. Advanced materials, modeling, and monitoring are necessary to avoid these events. Self-healing composites can provide new avenues to fatigue-tolerant blades [39,40] (see Fig. 10-5).

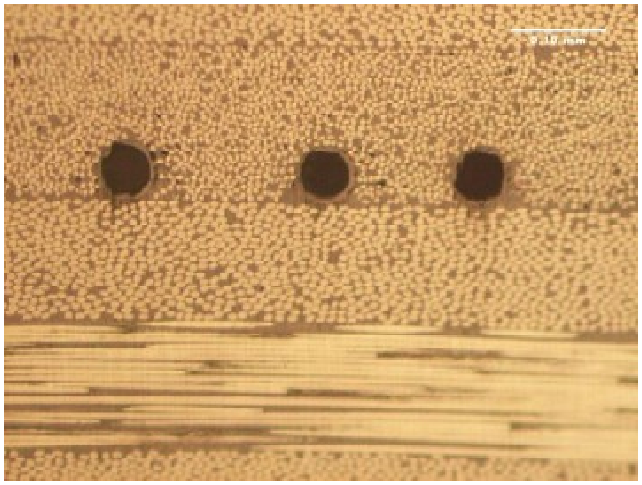

Figure 10-5 Bio-inspired self-healing can be achieved with hollow 35-micron diameter glass fiber embedded in a carbon-fiber reinforced laminate. Uncured resin within the fiber released by mechanical damage infiltrates the damage site and restores mechanical integrity [40]. Source: I. Bond, University of Bristol, UK.

6. Research Directions

Superconductors. The present generation of superconductor wires (yttrium barium copper oxide [YBCO] films on textured substrates, the so-called coated conductors) have been optimized primarily for low-field 77 K power cable applications. Their use in high-power-density rotating machines requires increased current in several Tesla fields in a conduction-cooled temperature range of at least 30 to 40 K. Critical current is controlled by the defect microstructure of the superconductor, and mechanisms that control critical current in these different operational ranges differ. A research first step is microstructural study of a variety of materials prepared with different deposition parameters. The microstructure needs to be related to current density and theoretical models developed. This is the classic triangle of materials science: processing — microstructure — properties. An understanding of the mechanisms opens up new routes to processing, including artificial layering, impurity doping and nano-defects, control of disorder, and reduced intrinsic anisotropy. Controlling grain boundaries is another key to facilitating current flow and relaxing texturing requirements in YBCO-based wires.

High-Strength, Self-Healing Composite Materials and Structures. Fatigue- and impact-tolerant material studies are required to produce optimum, high-load structures. To avoid the catastrophic cost of unscheduled offshore maintenance, highly accurate predictive models and condition-based monitoring are required for the highly loaded composite blades. Many high-strength composites, such as carbon fiber-reinforced plastic used in aerospace applications, are used to only a small fraction of their strain to failure because they do not deform plastically. Self healing has the potential to overcome this limitation; such engineering approaches have been inspired by observing natural systems. Hollow glass fibers store agents for self-repair as well as provide reinforcement. A typical self-healing approach could take the form of fibers containing a one-part or two-part resin system [39]. Once selected, preferred materials would be characterized such that failure could be predicted based on load history. The predictive model would be compared to blade test data. A monitoring system would then be developed to provide the load history on the blade for comparison to the model, with the objective of predicting the useful lifetime.

7. Potential Impact

Superconducting generators enable a two- to three-fold improvement in torque densities of electromagnetic power conversion for wind turbines, producing larger and more efficient (half the loss) power generation equipment. With the addition of optimized materials for large wind turbine structures, this will permit the cost-effective fabrication of 10-MW class and larger wind turbines. Major efforts are already underway in Europe to address the offshore wind power market with high-rating, direct-drive superconductor generators and a new generation of blades. Advanced materials for power generation and conversion developed in the United States will enable a U.S.-based wind turbine industry providing a new major source of cost-effective, large-scale renewable power, and potentially, a major new export industry. This technology is the key enabler for achieving high penetration of offshore wind power in the United States. This same technology will enable broad application across the entire field of rotating machinery — utility and hydro-generators, industrial motors, and propulsion motors for transportation.

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Chapter 11: Panel 9 — Scientific User Facilities
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I. INTRODUCTION

The Scientific User Facilities (SUF) stewarded by the Department of Energy's (DOE's) Office of Basic Energy Sciences (BES) are a national treasure and have no equal anywhere else in the world. Collectively, the SUF staffs possess a wealth of scientific knowledge, the capabilities offered are truly world-class, and the facilities encompass a broad geographic spread. The SUFs constitute a unique resource for the characterization of materials and chemical processes at the highest levels of spatial, spectral, and temporal resolution, as well as the synthesis and exploration of matter at the nanoscale.

While the scientific productivity of the SUFs is unmistakable, there are many opportunities to enhance their impact in achieving DOE's mission, especially as it relates to bridging the gap between basic and applied research in clean energy technologies. The SUFs hold significant untapped potential for fostering innovation and economic competitiveness, including within U.S. industry and in collaborations between industry and basic researchers. The Panel on SUFs proposed a coordinated effort to target energy research areas identified by the Workshop. Specific recommendations are the following: (1) enhance industrial outreach by SUFs with a systematic and sustained effort to engage targeted sectors in the clean energy industry; (2) review and consider modifications of existing policy and priorities for SUF user access to encourage industrial use and provide incentive for both industry and SUFs to develop a mutually engaging relationship; and (3) develop capabilities for (a) experimentation on materials/devices under real world conditions and at a realistic scale; (b) characterization of new materials with rapid-throughput methods to accelerate discovery; (c) extension of the limits of spatial, spectral, and temporal resolution; and (d) validation of theory/modeling/simulations.

II. OVERVIEW OF SCIENTIFIC USER FACILITIES

The BES-stewarded SUFs provide key technical tools needed for 21st-century science in basic and applied energy-related disciplines. Full details can be found in Ref. 1.

As shown in Fig. 11-1, the SUFs include synchrotron radiation sources, neutron sources, electron microscopy centers, and nanoscience centers. Thousands of scientists conduct their research at these state-of-the-art facilities each year, advancing the knowledge base of the underlying physical processes, chemical reactions, and materials properties that comprise our scientific understanding of energetic phenomena. Researchers from academia, national laboratories, and industry are free to access these facilities primarily through a merit-based peer-review system. The facilities are on a large scale and require resources to build and operate that are well beyond those of individuals, groups of individuals, or even most institutions and companies.

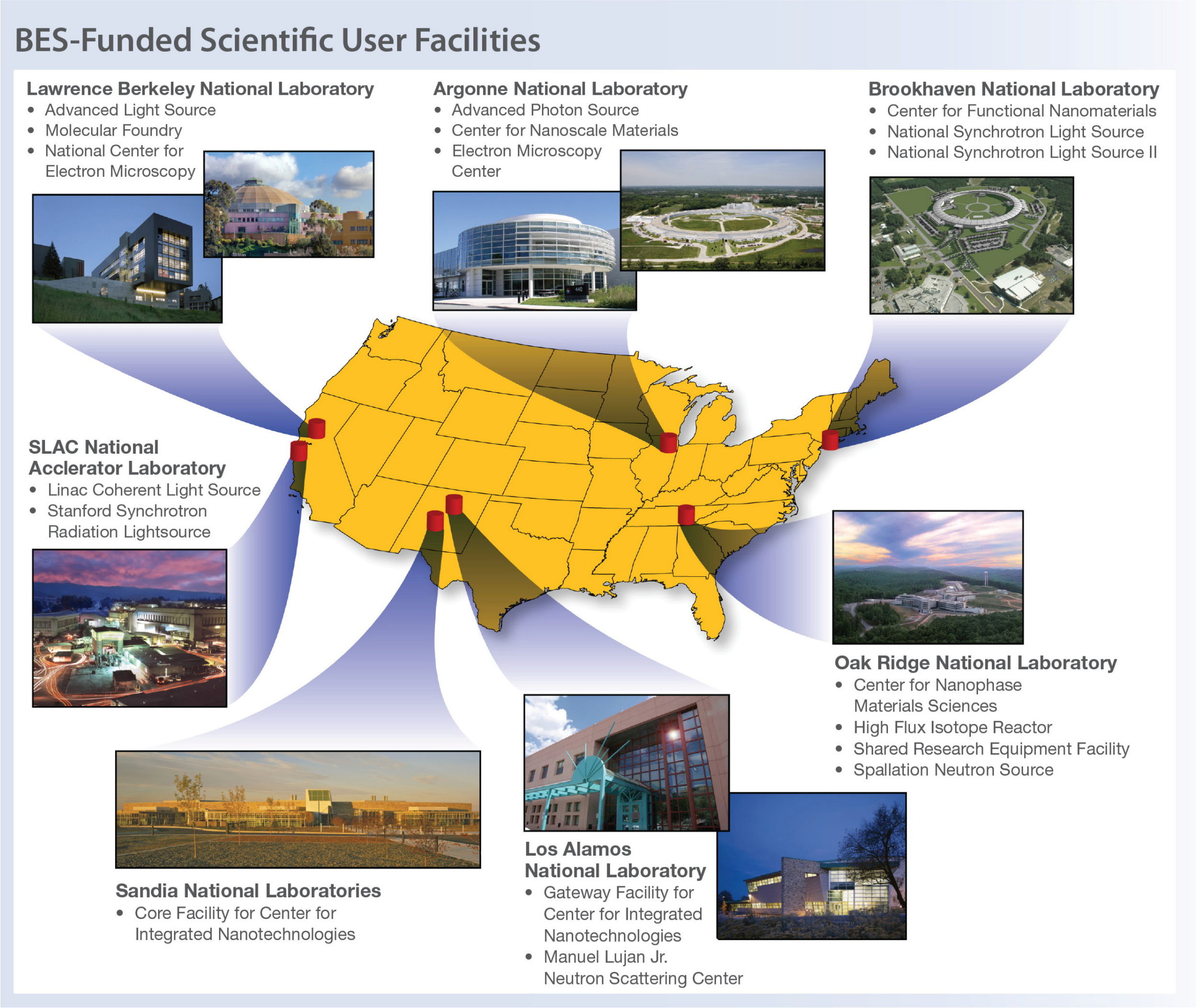

Figure 11-1 Location and descriptions of the SUFs stewarded by BES

The synchrotron radiation (photon) sources, neutron sources, electron microscopy centers, and nanoscience centers each have a specific role to play in furthering energy research. For example, today's synchrotron "light source" facilities produce X-rays that are millions of times brighter than those available in laboratory settings. Scientists use these highly focused, intense beams of X-rays to reveal the atomic structure in a wide range of materials, including metals, semiconductors, ceramics, polymers, catalysts, plastics, and biological molecules. The wavelength can be selected over a broad range to match the experimental need. With these and additional features, such as controllable polarization (both linear and circular), coherence, and ultrafast pulsed time structure, synchrotron radiation is the X-ray source of choice for a wide range of materials research.

The neutron sources provide a versatile probe of the atomic and molecular arrangement, motion, and magnetism in materials. Neutrons penetrate through many centimeters of a solid and so can determine the material structure in-situ or provide radiographs of technological devices such as engines and batteries under operating conditions. They have unmatched sensitivity to hydrogen and other light elements and can distinguish different isotopes of the same element.

The nanoscale science research centers provide facilities, equipment, and expertise for synthesis and study of materials at the nanometer scale—probing single atoms, clusters of atoms, and molecular structures. The scientific theme of these centers is to observe, understand, and predict how these nanosystems function.

Finally, the electron beam micro-characterization centers provide access to cutting-edge instrumentation for direct imaging and micro-analysis of materials at the atomic and molecular level. In many cases these instruments now incorporate in-situ environmental capabilities such as gas reaction, tensile, or ion bombardment chambers. Advances in specimen preparation have enabled the atom-level analysis to take place at specific sites in technological materials. These instruments provide structural and chemical information over critical length scales complementary to those probed with neutrons and X-rays.

III. PRIORITY CAPABILITY DEVELOPMENT

The Workshop Panel on Scientific User Facilities recommended the following capability development at the SUFs to optimally impact the priority research directions (PRDs) of this report:

1) Experimentation at scale on materials/devices under real world conditions

An essential bridge between basic science and applied research is the study of devices, products, materials, catalysts, etc., under their operating conditions to ensure that results relate to actual device performance. This study might necessitate collecting data at high or low extremes of temperature, at high pressure, in the presence of gases or liquids, and/or at operating voltages in a working device. The SUFs may need to handle full-scale devices, ranging from a solar panel to a battery that powers a hybrid locomotive. X-rays, neutrons, and in-situ electron capabilities are well-suited for these "real world" studies.

2) Tools for characterization of new materials with high-throughput capabilities

Breakthrough discoveries of materials are needed in many energy fields, and these materials must possess properties specifically tailored to a given application, e.g., new catalysts, photovoltaic materials, and superconductors. Materials discovery can benefit from coordinated use of experimental characterization capabilities and knowledge gained at the nanoscience centers and photon, neutron, and electron facilities. Capability for high-throughput testing is particularly important in the search for new materials.

3) Studying and imaging of interfaces and interfacial phenomena at all length scales

Interfaces play a key role in solar photovoltaics, carbon sequestration, advanced lighting, biofuels, batteries, and other energy technologies. These interfaces are typically heterogeneous and complex, and structural and physical information needs to be determined over multiple-length scales from centimeters to nanometers, even to atomic resolution. The full arsenal of SUF techniques and capabilities should be employed to address this scientific challenge.

4) Techniques for high spatial, spectral, and temporal resolution

Many critical needs of energy research require even higher spatial, spectral, and temporal resolution than available today. An example is the need to image with nanometer spatial resolution the electrode structure/chemistry within one nanometer of battery interfaces, combined with one-millisecond time resolution during the charge/discharge cycle. Improvements are needed in everything from detectors to beam optics, and even in the facilities themselves.

5) High-quality experimental input for theory, modeling, and simulation

Much development of advanced materials for energy applications now relies increasingly upon theory, modeling, and simulation, since relying solely upon producing and testing new materials simply takes too long. In other cases, such as carbon sequestration and nuclear waste storage, the time periods of interest are much too long for experimentation. Throughout energy technology, there is a need for prediction of component behavior under actual and extended life conditions. The unique SUF capabilities could generate high-quality data to feed into theory-modeling-simulation efforts. This requires SUF users to be well-connected with modelers and theoreticians. The SUFs are particularly well-suited for this type of research, since they could have excellent capabilities to handle real-world samples (see item 1 above), produce high-quality data, and if necessary, can run relatively long experiments.

The topics summarized in Table 11-1, derived from the research needs of the other eight Workshop panels, are areas where SUFs could have a major impact. A recommendation is to hold a series of focused workshops for each specific energy community with SUF scientists to match community needs with SUF capabilities and detail these opportunities.

Table 11-1 Targeted energy research areas from the PRDs of the other panels where research at SUFs could have significant impact

Solar

- Tools to understand the optical, electrical, mechanical, and chemical properties of heterogeneous interfaces
- Methods to characterize interfaces and then to compare results to computational models
- Studies of photochemistry and photochemical degradation
- Analytic tools for failure analyses
- Studies of stoichiometry and defect chemistry control of multinary inorganic semiconductors
- Atomic and micro-scale structural studies of large scale systems (solar modules): how do we characterize materials; how do we handle the data?

Advanced Nuclear

- Experimental characterization, irradiation, and modeling of a prioritized set of controlled materials in multiple environments
- Studies of actinide and fission product behavior (research that transcends technology choices/policy decisions)
- Studies of f-element electronic structure and bonding
- Synchrotron beamline experiment with environmental capabilities (e.g., high-temperature water)
- New facility to perform nanoscale testing and characterization of irradiated materials

CO_2 Sequestration

- Studies of CO_2-water-rock interactions, and use of geochemistry and/or biogeochemistry to accelerate plume stabilization and trapping mechanisms

Electricity Storage

- Forefront in-situ and ex-situ tools to probe interfaces
- Novel energy storage architectures with tunable energy density/power performance via structure-property relationships, with understanding of these relationships at all length scales

Electric Power Grid Technologies

- Atomic level control of the microstructure of high-temperature superconductor films on textured substrates for higher pinning and reduced grain boundary limiting
- Atomic level control of nanoparticle fillers, dispersions, and interfaces
- Improvement of power electronic materials such as SiC

Advanced Solid State Lighting

- Fundamentals of molecular interactions between organic light-emitting diode hosts, guests, interfaces, impurities, contacts, and environment that limit reliability

Table 11-1 (Cont.)

Biofuels
• Methods of imaging and spectroscopy to characterize bulk and surface diffusion (e.g., of enzymes on lignocellulose) under realistic processing conditions
• Relation of catalyst/enzyme properties to performance for catalyst development
• Atomic-level control of catalyst/enzyme structure
• Approaches to anchoring or tethering metals to supports to minimize leaching
Efficient Energy Generation and Use
• Understanding anion/cation doping, e.g., in zirconates, titanates
• Studies of perovskites and spinels that promote O_2 exchange and reduction at gas and oxide interface
• Studies of oxidation-reduction reaction performance and degradation over various catalysts in acid systems
• New materials directions: core/shell materials, preferentially faceted nanostructures

IV. IMPACT ON ENERGY RESEARCH

Examples presented in this section illustrate how world-class energy-related research is already being conducted at the SUFs, often by industry or in collaboration with industry. These examples coincide with the scientific areas in Table 11-1 and the enhanced SUF capabilities described above.

A. Nanoscale Imaging of Catalyst Chemistry (Advanced Light Source, Lawrence Berkeley National Laboratory)

The performance of catalysts for biofuel synthesis depends on a complex mix of interactions with substrate, reactants, and products. But structural and chemical characterization under reaction conditions is lacking; in some cases, even the active catalyst is unknown. At Beamline 11.0.2 of the Advanced Light Source (ALS), a scanning transmission X-ray microscope (with nanoscale resolution) is combined with a “nanoreactor” chamber to measure nanoscale chemical contour maps, allowing analysis of chemical species before, during, and after reaction. This promising tool can be used in the quest to design and tailor catalysts for maximum efficiency (see Fig. 11-2).

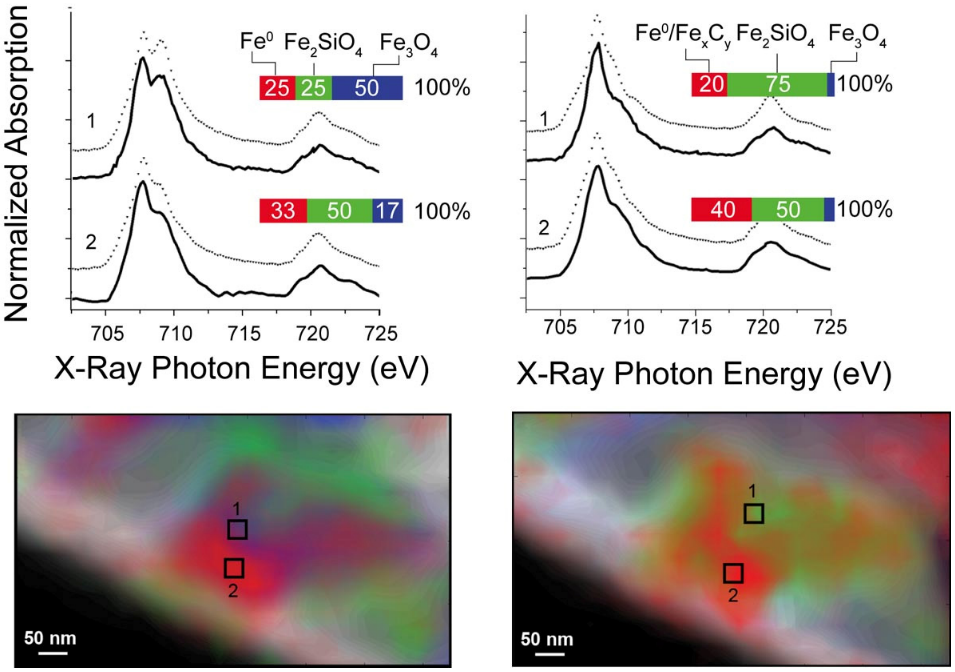

Figure 11-2 Tracking changes in an iron-based catalyst at ALS. Top left: Iron $L_{2,3}$ spectra taken before catalysis from two regions (1 and 2) of the catalyst material after 2 hours in hydrogen at 350°C. Top right: Spectra after catalysis in synthesis gas at 250°C for 4 hours. Dotted lines are fits by linear combination of reference spectra. Bar graphs represent calculated relative percentage of different iron phases at the sampling points. Bottom: Iron species contour maps generated from spectra taken at each pixel, with colors keyed to bar graphs above.
Source: [2].

B. 3-D Microstructure Visualization and Modeling of Deformation in Metal Matrix Composites (Advanced Photon Source, Argonne National Laboratory)*

Ongoing research by industrial users employing the micro-tomography system at the Advanced Photon Source will support U.S. efforts to make lightweight connecting rods for passenger cars by (i) visualizing and quantifying the fraction and distribution of SiC, pores, and Fe-rich inclusions, (ii) understanding the role of Fe-rich inclusions and pores on tensile and fatigue resistance of metal matrix composites, and (iii) quantifying the degree of damage as a function of distance from the fracture plane. This technique will also have application in CO_2 sequestration and in the design and operation of new materials for advanced nuclear power plants.

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* Courtesy of N. Chawla, Arizona State University, in collaboration with Alcoa, Ford, GM, and Chrysler.

C. In-situ Studies of Industrial Batteries (National Synchrotron Light Source, Brookhaven National Laboratory)*

As advanced battery technologies progress toward large-scale application, an in-depth understanding of their complex chemical processes, degradation pathways, and failure modes in full-scale cells is required but is limited at present by the traditional inaccessibility of the batteries' active components during cycling. GE Global Research, in partnership with Rutgers University and Brookhaven National Laboratory, is using the high-energy (60–160 keV) X-ray diffraction at the National Synchrotron Light Source (NSLS) to study the electrochemical processes in the sodium metal halide batteries that GE is currently commercializing. The polychromatic X-rays at this beamline provide the best combination of penetrating power, measurement speed, and spatial resolution of any diffraction technique, especially for studying deeply buried processes like those in the sodium cells. Energy dispersive X-ray diffraction yields the ability to spatially and temporally characterize full-size cells as a function of time, cycling, temperature, etc. This capability enables direct feedback into the battery design optimization process, and helps validate and inform theoretical models. (See Fig. 6-5.)

D. Organic Solar Cells: Importance of Molecular Mixing (Stanford Synchrotron Radiation Laboratory)

Organic photovoltaics show promise for low-cost flexible solar cells that are being manufactured by companies such as Konarka and Solarmer Energy. These cells consist of an active layer of a phase-separated mixture of a polymer (electron acceptor) and fullerene (donor). Optimization is largely done empirically, with some mixtures optimized at a 1:1 polymer:fullerene ratio, others at 4:1. The reason for this difference is unclear. X-ray diffraction at Stanford Synchrotron Radiation Laboratory was used to characterize polymer/fullerene molecular packing in blends optimized at 4:1, and revealed the surprising formation of an intercalated or intimately mixed bi-crystal [3,4]. These studies will help enable more rational optimization of solar cell processing and materials.

E. Small Angle Neutron Scattering (SANS) Studies of Nickel-Based Superalloys (High Flux Isotope Reactor, Oak Ridge National Laboratory)†

Waspaloy™ is an ultra-high-strength nickel-based superalloy used in hot-section components of turbine engines for power generation. Solid precipitates or inclusions in Waspaloy's microstructure stop crack propagation. Researchers used the general-purpose SANS at the High Flux Isotope Reactor to analyze how repeated heating and cooling cycles affect Waspaloy inclusions. They found that precipitate distribution, which has a direct bearing on mechanical properties, changes as a result of repeated thermal exposure/cycling during service. The measurements show clear trends in the increasing correlation distance between precipitates as a function of ex-situ heat treatment. The material's electrical response changed as cracks formed.

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[*] Courtesy of E. Hall, General Electric Global Research.

[†] Courtesy of Rosario Gerhardt and Ricky Welchel, Georgia Tech, and Ken Littrell, Oak Ridge National Laboratory

This information will enable development of better monitoring techniques to catch flaws before they lead to failure, which will lead to more reliable and longer lasting turbines for power generation.

F. Improved Hybrid Solar Cells via In-situ UV Polymerization (Center for Nanoscale Materials, Argonne National Laboratory)

One approach for inexpensive inorganic–organic hybrid photovoltaic cells is to fill highly ordered titania (TiO_2) nanotube arrays with solid organic hole conductors such as conjugated polymers. Using an in-situ ultraviolet (UV) polymerization method developed at the Center for Nanoscale Materials for growing polythiophene (PT) inside electron-accepting TiO_2 nanotube arrays (see Fig. 11-3), researchers achieved significant performance improvements: strong coupling at the polymer–oxide interface, important for efficient exciton separation, and fewer conformational defects, facilitating hole transport. Compared with the reference device infiltrated with pre-synthesized polymer, the UV-PT cell shows a factor of >10 increase in photocurrent.

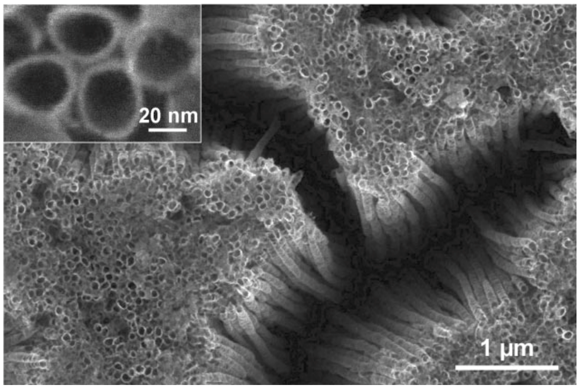

Figure 11-3 Field emission scanning electron microscope images of a TiO_2 nanotube array top surface after annealing. Inset shows a zoomed view of the nanotubes with 30-nm inner diameter and wall thickness of 5 nm. Source: [5].

G. Silicon Nanowire Architecture for Photovoltaic Applications (Center for Integrated Nanotechnologies, Albuquerque, New Mexico)

A new project entitled Assessment of Silicon Nanowire Architecture for PV Application is being conducted at the Center for Integrated Nanotechnologies (CINT) in collaboration with Sharp Laboratories of America, with the goal of assessing fundamental barriers to solar energy harvesting by semiconducting nanowires. It addresses several key science issues related to the manufacturability of silicon nanowire devices for solar cell applications (see Fig. 11-4). The objective of the nanowire approach is to obtain high efficiencies, similar to crystalline Si photovoltaic efficiencies, at low costs, approaching those for thin film processes. The project builds on the strength of nanowire synthesis and integration science developed at CINT.

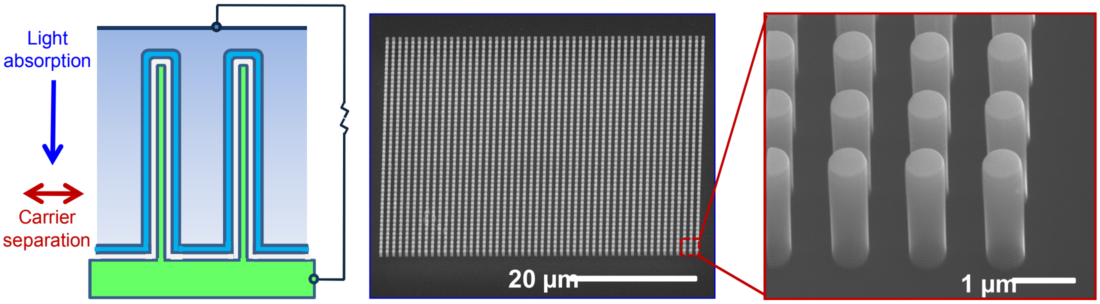

Figure 11-4 Schematic of radial nanowire device (left side). Scanning electron microscopy image of an ordered array of Si nanowires (center and right side). Source: S. A. Dayeh and S. T. Picraux, Center for Integrated Nanotechnologies (CINT), Los Alamos National Laboratory, unpublished.

H. Single Atom Imaging of Industrial Nanocatalysts (National Center for Electron Microscopy, Lawrence Berkeley National Laboratory)

At the National Center for Electron Microscopy, catalytic processes are studied with atomic resolution and single-atom sensitivity. A project with Haldor Topsøe is investigating the industrial nanocatalyst molybdenum disulfide (MoS_2), which is used for oil refinement, hydrogen evolution, and photo-oxidation. A structural identification on a single-atom level of catalytically active sites at the edge of MoS_2 crystals has been achieved with transmission electron aberration-corrected microscopy (Fig. 11-5).

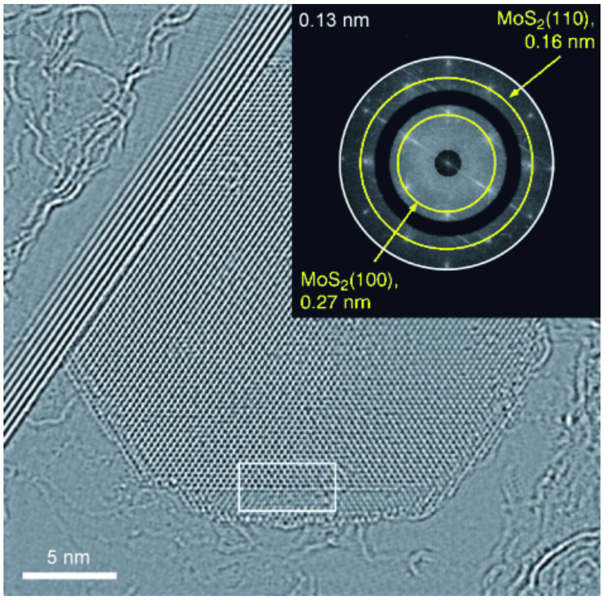

Figure 11-5 Image of a MoS_2 nanocrystal supported on graphite, taken with a transmission electron microscope, which provides state-of-the-art optical corrections for spherical aberration (blurring). The inset is a fast Fourier transform of the image and shows distinct 0.27 nm and 0.16 nm lattice distances corresponding to the MoS_2 (100) and (110) lattice planes, respectively. Image Fourier components of the graphite support are filtered out. Source: [6].

While these examples show SUFs already playing a role in energy-related research, this research is still predominantly being performed by academia and national laboratory scientists. The current percentage of ***all*** industrial research at these facilities is small (<6%), and the percentage of research by ***energy-related*** companies is most likely a small fraction of this total. It would be desirable to monitor industrial energy-related involvement at SUFs systematically and to introduce a new metric of research conducted at the SUFs: "energy-related" research involving industrial users or partners.

In fact, the percentage of industrial usage of synchrotron and neutron sources has been steadily decreasing from the highs of almost 20% in the early 1990s (Fig. 11-6), although the total ***number*** of users has increased substantially over this same time period. The actual number of industrial users is plotted in Fig. 11-7; it has remained relatively constant over the last decade, with only one period of significant growth.

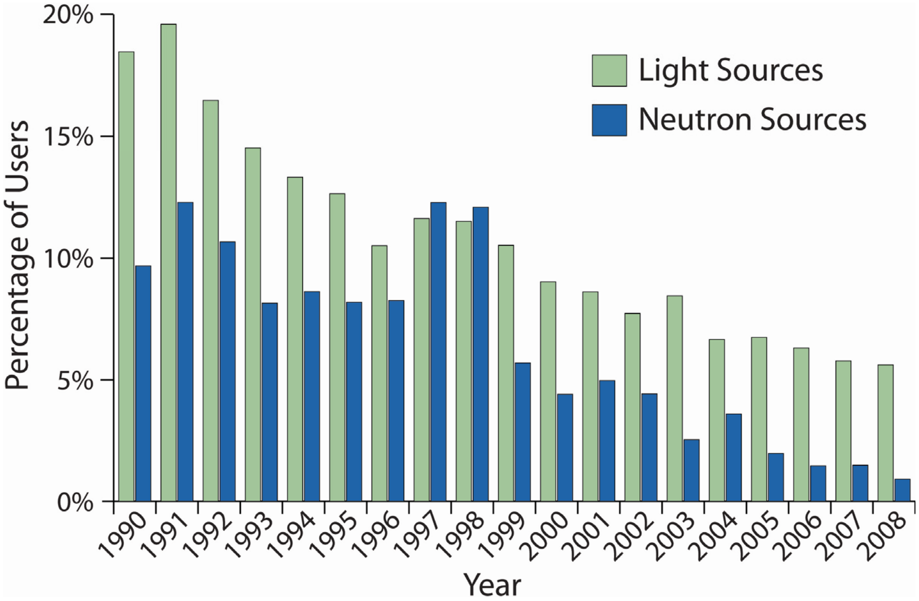

Figure 11-6 Percentage of industrial users of the synchrotron and neutron SUFs from 1990-present. Source: BES Annual Facilities Questionnaire.

The low industry participation (and, specifically, the energy research industry) may result from lack of knowledge of the SUFs (and indeed of DOE-BES as a whole) and their capabilities, but also from the special needs of the industrial research community (see Appendix in this chapter) and the lack of a directed program in this area at the SUFs (see recommendations in Section VI).

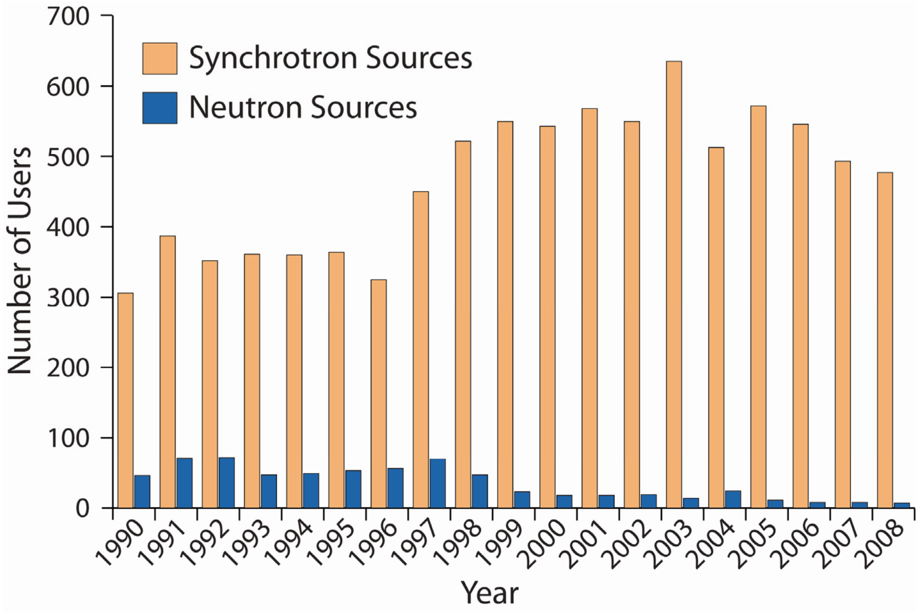

Figure 11-7 Number of industrial users of the synchrotron and neutron SUFs from 1990-present. Source: BES Annual Facilities Questionnaire.

V. ENGAGEMENT OF USER FACILITIES WITH INDUSTRY

As described above, the DOE-BES SUFs provide a comprehensive suite of powerful experimental tools. The open and transparent policy for user access has led to the utilization of SUFs by thousands of researchers annually from academia, government, and industry to conduct research in a wide range of basic and applied sciences. Over the last few years, energy research has become a significant part of the research conducted at SUFs, as the awareness of the nation's energy problem as well as available research funding has increased. Today, the majority of the energy research carried out at SUFs is focused on discovery and use-inspired basic research, although there is an increasing awareness of the importance of applied and industrial research.

Based on the input from Workshop attendees, there is clearly a lack of knowledge of the capabilities available at the SUFs by many industrial researchers, and a significant barrier for industrial researchers to integrate the utilization of SUFs into their research and development programs (see Appendix). Conversely, SUF researchers often lack awareness of the most critical research needs of industry. Thus, the well-known gap between basic and applied research also manifests itself in the utilization of SUFs. This shortcoming is illustrated by the limited number of collaborations across the basic and applied boundaries on the same technological problem, even in cases where both types of research are conducted at the same SUF, and the often very long periods of time it takes for a relevant experimental result or technique developed from basic research to help solve a technological problem.

Some industrial access models that served the SUFs well in the past will no longer work in the 21st century. Previously, large industrial research laboratories were willing to invest significant staff time and money to operate instruments at SUFs, and their researchers pioneered many of the experimental techniques used today for basic and applied research (see Fig. 11-6, showing the relatively high percentage of industrial users in the early 1990s). However, industrial research has become increasingly focused and cost-conscious. Advances in instrumentation, modeling, and computing have led to the expectation of rapid and targeted data generation and analysis. Global companies now seek the most accessible, turnkey, and low-cost capabilities anywhere in the world. This new paradigm poses challenges that BES should address.

The Panel believes that the SUFs could build on their success and play an important role in bridging the gap between basic and applied research, complementary to efforts underway at DOE's Energy Research Frontier Centers and Energy Innovation Hubs. Specifically, we propose a coordinated effort to take full advantage of the unique environments created by SUFs and to maximize SUF utilization in targeted energy research areas, such as those in Table 11-1.

For a given targeted area, the effort should include the following:

- Expand SUF outreach efforts to industry in the targeted area;
- Analyze potential SUF contributions to the targeted area with a focused group of researchers; and
- Organize regular meetings/workshops to bring together researchers in the targeted area, identify specific research projects, form teams of collaborators, and suggest SUF instrument upgrades.

This effort would bring together researchers who "own" the problem and researchers who know the tools, prepare the researchers properly for a sustained and productive interaction, and support them with the investment BES is making at SUFs. Essentially, this effort involves making the whole SUF system a resource available to the targeted areas of research in the most efficient way.

VI. RECOMMENDATIONS

Panel 9 at the BES Advisory Committee Workshop on Science for Energy Technologies formulated the following recommendations to help the SUFs substantially impact the DOE energy mission. The recommendations should not significantly detract from the SUF focus on basic science driven primarily by academia and national laboratories. The strategic imperatives to diversify the U.S. energy portfolio and to lay the technological foundation for the 21st-century economy make the goal of engaging the SUFs more broadly in the science of clean energy technology both worthwhile and timely.

Recommendation 1: Enhance industrial outreach by SUFs and develop a systematic and sustained effort to engage targeted industrial sectors.

- Expand current SUF outreach activities. Possibilities include establishing a specific website at each SUF targeted toward industrial users, attendance at targeted industry-sector specific conferences, and other such outreach activities.
- Promote networking among the SUFs to jointly achieve broad market coverage for industrial energy research.

- Identify needs of targeted industrial sectors by engaging industry and all SUFs. Consider periodic 1-2 day workshops where a group of SUF researchers addresses an industrial sector, such as solid state lighting or advanced nuclear energy, highlighting specific capabilities of SUFs focused on the targeted sector. They would be highly interactive, informative, and problem-oriented. The goal would be to develop active, team-oriented collaborations. An example of successful fostering of collaborations was the workshop, Energy Storage Research Opportunities at the National Synchrotron Light Source, sponsored by the Joint Photon Science Institute, at Brookhaven National Laboratory in June 2009 (see Appendix).

- Develop industrial consortia to access SUFs. These consortia would be facilitated by one or more of the SUFs and act as a resource of information and know-how for industrial problem solving.

- Coordinate activities across all SUFs. This task could avoid unnecessary and potentially costly duplication of effort. A single SUF may not be able to act as a one-stop shop to solve an industrial research problem; access across multiple SUFs may be required. Given the different procedures at each SUF, there is the potential for wide variability in how these recommendations may be implemented. Most issues are complicated by differences in activities related to SUF policies and procedures, such as meeting industry science needs, gaining access to facility time, and publishing results. A uniform approach for all SUFs to the extent possible, coordinated by BES, would be desirable, although significant differences in the modes of operation of different SUFs must also be recognized.

Recommendation 2: Review and consider modifications of existing SUF user access policy and priorities to meet industrial research needs and encourage use, and review and modify DOE policies to provide incentive for both industry and SUFs to develop a mutually engaging relationship.

- Develop industrial access policy.
  - BES and SUF directors should explore ways to enhance appropriate industrial research participation at their facilities. Access policies could be developed that address the barriers to industrial participation. For example, setting aside a modest fraction of specific capabilities for "quick response" projects from industry and basic science users could help to address one barrier to industrial participation — the need for rapid turn-around. The specific allocation details should remain at the discretion of the facility director. See as an example the NSLS guidelines in Ref. 7.
  - Criteria used to evaluate research proposals submitted by industrial/applied research users, while still emphasizing scientific merit, should also weigh technological excellence and impact on DOE mission objectives. An example is the recent NSLS proposal evaluation rubric, which includes "technological merit" as an explicit scoring criterion. Proposal review panels should include industrial peers.

  - Avenues should be explored for continued and regular access to SUFs for those users who need extended and sustained use.
  - SUFs are encouraged to have a full-time industrial liaison. In some cases it might be useful to consider developing a service-oriented group. The industrial liaison would act as the first point of contact with the industrial user and would strengthen, enhance, and help coordinate the industrial research. Ideally, the liaison would speak the language of an industrial researcher.
  - SUFs should explore providing services above and beyond those that they currently offer, including consultation to aid the industrial researcher in identifying the best technique for the problem, in writing a proposal for access, and in experiment planning, data collection, and data interpretation.
  - SUFs could provide free first-time analyses for straightforward industrial research problems.
- Develop access models for industrial users.
  - Improved access models should continue to be investigated to allow and promote industrial users long-term access to facilities at the SUFs (see Table 11-2). There is a track record of success of companies partnering as stakeholders in the development and operation of beamlines at synchrotron radiation sources leading to discovery and innovation. For example, the contributing/partner user model is highly successful and should continue.
- Develop workhorse capabilities.
  - Several techniques (e.g., X-ray diffraction, extended X-ray absorption fine structure, photoemission spectroscopy, and small-angle X-ray scattering) have become workhorse techniques in the existing industrial user community and are in high demand. It would be desirable for BES to establish a suite of such capabilities that are state-of-the-art, fully staffed, with high-throughput capabilities, and remotely accessible. The prioritization of these capabilities could be facilitated using a program advisory committee that would have some industrial participation, with guidance from user statistics to validate the choice of beamline suite.
- Establish advisory committees.
  - Each SUF should include at least one industrial researcher on their Scientific Advisory Committee.
  - Each SUF user organization should include at least one member from industry.
  - An Industrial Program Advisory Committee should be established at each SUF with an enhanced industrial access program.

- Examine new models for intellectual property (IP) protection for engaging with U.S. industry.
  - The IP complexity of academia/national laboratories working with industry is not new, and detailed recommendations are outside the scope of this report (see also Chapter 2). More flexibility and simplification of DOE policies regarding IP issues are desirable to facilitate industrial usage of SUFs.
- Improve cost model.
  - The current model of calculating full-cost recovery for proprietary time at SUFs, a "one-fee covers all" approach, could be made more flexible with a graded cost structure based on the capability of the experimental equipment and/or fee per sample/analysis. Again, details are outside the scope of this panel, but this is a critically important area and needs to be revisited.
- Improve SUF access requirements.
  - Uniformity in the access requirements for an industrial researcher to the suite of SUFs is highly desirable. There is a barrier perceived by industry to initiating research at an SUF due to the overwhelming administrative burden arising from different requirements for access, safety, proposals, training, and badging, to name a few.
- Establish incentives.
  - Incentives and recognition could be established to encourage SUF management and staff to interact and collaborate with industrial users.

Recommendation 3: Current capabilities: Develop experimental capabilities to allow experimentation on real materials/devices under real world conditions with imaging at all length scales to drive innovation in the development of new materials.

(see section on Priority Capability Development)

Recommendation 4: Future capabilities: Push the limit of SUF capabilities for high spatial, spectral, and temporal resolution to meet the increasingly sophisticated measurement needs for the discovery and development of materials and chemistries for next-generation energy systems and technologies.

(see section on Priority Capability Development)

In conclusion, the BES-stewarded SUFs can play a major role in solving challenging and timely scientific problems underlying energy technology, such as those detailed in this report. They are well suited to engage with industry in bringing new energy technologies to market, which will address critical national energy needs as well as create jobs and spur future economic growth. The scope of the SUFs is beyond that which can be maintained by an individual industrial concern. The current participation rate by industry is low (6%), and it behooves BES to reach out and develop mechanisms to further engage the vibrant industrial research community in SUFs.

Table 11-2 SUF access model

Access Type	Details
General User	2-year proposal; some limited rapid access; peer-reviewed; allocated by panel
Participating research team/ Collaborative access team	Design, construct, maintain, operate, and manage beamline; approved by Scientific Advisory Committee and Chair; renewable every 3 years; complete control of equipment and program; guaranteed 75% of beamtime; expensive; needs consistent funding & staff
Contributing user /Partner user	Enhance beamline capabilities and/or contribute to operation of facility beamline; guaranteed up to 50% of beamtime; some control over instrumentation and beamtime; less expensive than a participating research team
Proprietary user	Approved by Chair; full-cost recovery in exchange for full ownership of intellectual property
Special arrangements	Service contracts, etc.

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APPENDIX

Industrial Research Needs

"Industrial research needs" is a catch-all phrase that does not begin to capture the complexity of industrial SUF-user community needs. Industrial research covers a wide spectrum: from a small company with a single research focus to a large global corporation with a diverse and large research portfolio; from a problem that requires an immediate answer due to a manufacturing or production issue to a long-term research problem; from a single sample to hundreds of samples; from a problem which involves a known technique to one where new SUF analytical capabilities need to be developed. No single solution will meet all industrial research needs. Flexibility and a range of possible solutions are required.

For the scientific information obtained at an SUF to have the desired impact on an industrial research program, certain attributes are typically required. In some cases, these may differ from those of a comparable national laboratory or academia-led research program:

- **Timeliness -** Industrial research efforts tend to be short (months to few years). For example, a technology delivery project will have monthly milestones. Issues with a manufacturing plant need to be addressed, ideally within days or even hours. This situation necessitates very timely access. Moreover, if particular tools/techniques have a demonstrated benefit to a research project, access may be needed on a regular basis to continuously add value, particularly for process development or reliability assessment.

- **Quality -** Data must be reliable and reproducible; so equipment must be calibrated, in good working order, and consistent, with metrics recorded and available.

- **Expertise -** Industrial research is usually conducted by multidisciplinary teams with the individual researcher having to engage in all aspects of the problem. Moreover, a typical researcher will be involved in multiple projects at one time, often without continuity from one project to the next. These factors contribute to the industrial researcher lacking the time to become an expert in a particular SUF technique; this situation is particularly true for smaller companies with a small research staff. Significant mentoring by SUF staff is, therefore, likely required.

- **Problem Focus -** Industrial research is typically problem-oriented, and relevant data must be focused on that problem rather than on peripheral issues. For complex problems, it is unlikely that a single technique at a single SUF will suffice; so the researcher may need access to a suite of tools at several SUFs.

- **Samples -** Data are most desirably obtained on the actual sample and devices, not on a model or ideal samples. Often data need to be obtained on many samples, comparing some physical or chemical property as a function of some process condition.

- **Geographic Access -** Travel budgets are under constant pressure. Industries will take geographic location into account when choosing an SUF.

- **Compatibility -** Certain methods and procedures are used by industry to ensure quality and compatibility, including ASTM and ISO methods. It would be advantageous if data obtained at an SUF adhered to some of these methods.

- **Publishing -** Often, industrial research results are not published in the open literature.

Example of Matching Industry Need with SUF Capability

A demonstration of fostering collaborations was through the workshop, Energy Storage Research Opportunities at the National Synchrotron Light Source in June 2009, sponsored by the Joint Photon Science Institute. The charge was to (1) demonstrate the ways that synchrotron and electron techniques can help solve important problems in this field and improve the understanding of characteristics and behavior of materials for the energy storage industry, (2) learn what the current issues are in energy storage from those performing research, and (3) produce two matrices of projects: one for action now at the NSLS, and the other to aid in planning for NSLS-II. The type of output from such a workshop is shown in Table 11-3 for the hypothetical case of battery storage. This table matches the specific needs in advanced battery research (columns) with capabilities at the NSLS (rows).

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Table 11-3 Matrix of synchrotron tools and technology issues in energy storage research. Source: Joint Photon Sciences Institute, http://jpsi.bnl.gov/events/energy/

ENERGY STORAGE MATRIX			Technology Issue				
			Electrochemical performance	Degradation mechanism during cycling and storage	New material for electrodes	Polymer/liquid electrolytes	Electrode-electrolyte interface (SEI)
Synchrotron Tool	Spectroscopy	EXAFS	Catalyst at interface	Local environment around specific element	Coordination and band length change		Element specific
		XANES	In-situ oxidation	Range reduction of valence changes	Redox reaction in-situ	Element selective ion complexing	Charge transfer process
		PES		Electronic energy-band structures			Bulk/surface electronic structure
		IR Micro-spectroscopy	Reaction pathway			Identify species present	Identify species present
	Scattering/ Diffraction	Single-crystal/ Powder XRD	Dynamic studies	Irreversible structural damages	Temperature dependent in-situ structure determination		Interface structure
		High-Energy XRD		Location specific structural changes in real batteries			
		μ-XRD			Phase transformations in micron region		
		PDF					In-situ time-resolved formation of nanoparticles
		SAXS/WAXS		Particle shape and size change	Particle evolution during cycling	Evolution of structures in real time at nano to micro scales	Formation of nano-particles/breakage of larger particles
		GISAXS/GIXD	Surface Structure			In-situ PEM structural changes	In-situ surface/ interface structure
		RXS/RXD			Element, charge and orbital ordering phenomena		
	Imaging	Micro-XCT	In-situ particles formation	Breakage 3D imaging during cycling	Morphological changes during cycling		Non-equilibrium Li battery
		TXM	Change in near surface morphology	Evolution of surface or interface structure at nano scale	3D elemental distribution at nano scale	Interface structure by phase contrast	3D imaging in nano spatial resolution
		SXM	Chemical states and local structure in micron scale	Oxidation state in micron region	2D composition and oxidation mapping		Local oxidation state change
		Topograph	Strain distribution near surface		Strain distribution		
		PEEM/LEEM	Surface element mapping		Surface 2D mapping		

Chapter 12: Conclusions and Recommendations

Many clean energy technologies today — e.g., solar photovoltaics, solid state lighting, batteries for plug-in vehicles, high temperature superconductor wires — are poised to advance with continuous innovation based on scientific understanding coupled with engineering, as well as with the disruptive discoveries that lead to more radical changes in energy technologies. In both cases, basic energy research has played and continues to play a central role in the innovation process. Basic energy research enables and accelerates the economic and technological transition by revealing the underlying principles controlling clean energy phenomena and translating this knowledge to industry. These innovations can significantly raise the operating performance of clean energy technologies and bring them to the tipping point of competitive viability with traditional fossil technology.

The DOE Office of Basic Energy Sciences (BES), with its broad-based fundamental research program in energy-related science and its unique user facilities, has a leading role in this scientific contribution to our clean energy future. To define the opportunity, the BESAC Workshop on Science for Energy Technology on January 18-21, 2010, brought together a broad cross-section of industry, national laboratory, and academic researchers to delineate the priority research directions that could resolve important technological challenges and to address barriers to effective implementation. A key conclusion of the Workshop was that while BES has done a good job of delineating broad foundational challenges in developing new energy technologies, there are specific scientific issues underlying roadblocks to performance in existing and emerging clean energy industries that could significantly accelerate the innovation process. These were outlined in a set of priority research directions. The second key conclusion was that direct, mutual engagement of BES and BES-funded researchers with industry is critical to achieve greater impact and accelerate the pace of innovation. The link to industry is essential in guiding the use-inspired science of BES-funded researchers, in cultivating interdisciplinary dream teams that include the best and brightest industry and BES-sponsored scientists, and in transferring key insights to industry. Key recommendations are:

- In addition to BES's commitment to support long-term grand challenge and discovery science, BES should work to extend the reach and impact of its programs to address some of the use-inspired science-based challenges identified at the Workshop that impede the development and adoption of clean energy technologies, and that are of particular interest to industry.

- BES and industry should foster stronger communication and more direct technical collaborations between their research communities. This direct engagement of BES-sponsored and industry scientists is essential for focusing basic research attention on key scientific issues that block development of clean energy technologies and for facilitating knowledge transfer to industry.

- BES-supported user facilities should seek to increase the level of industrial participation and use by considering refinements to its access policies, proposal selection criteria, and time allocations to more fully engage industry-based clean energy research; investigating how its existing and proposed beamlines and instrumentation could be adapted to the priority research directions and needs of industry outlined here; and engaging its beamline scientists and support staff to provide greater assistance to industrial users solving critical challenges in development and deployment of clean energy technologies.

Addressing these opportunities opens enormous opportunities to accelerate transformative solutions to the critical clean energy challenges we face and, at the same time, to promote the job growth and economic competitiveness we so urgently need for a sustainable and prosperous future.

The “Basic Research Needs” reports have become standard references in the scientific community and have helped shape the strategic directions of the programs funded by Basic Energy Sciences. **http://www.sc.doe.gov/bes/reports/list.html**

The report is available online at http://www.sc.doe.gov/bes/reports/list.html.

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