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National Postirradiation Examination Workshop Report

June 2011

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Idaho National Laboratory

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Idaho National Laboratory
Idaho Falls, Idaho 83415

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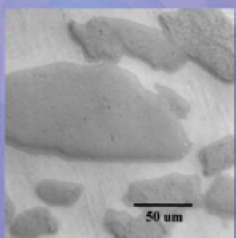
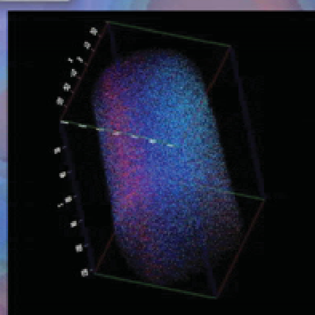
Postirradiation Examination

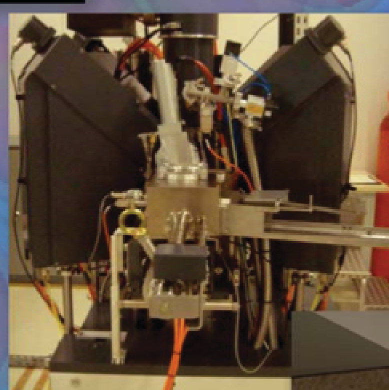
WORKSHOP WORKSHOP WORKSHOP

March 29-30, 2011
Gaithersburg, MD





WORKSHOP REPORT
June 1, 2011



U.S. DEPARTMENT OF ENERGY

Idaho National Laboratory INL

EXECUTIVE SUMMARY

Global energy consumption is expected to increase dramatically in the next decades, driven by rising standards of living and growing population worldwide. The increased need for more energy will require enormous growth in energy generation capacity, more secure and diversified energy sources, and a successful strategy to tame greenhouse gas emissions. Among the various alternative energy strategies, building an energy infrastructure that capitalizes on nuclear energy may enable a secure and clean energy future for the Nation.

On January 31, 2011, Peter B. Lyons, Acting Assistant Secretary for Nuclear Energy, approved Critical Decision (CD)-0, Approve Mission Need, for the Advanced Postirradiation Capability Project. As stated in the Mission Need, "*A better understanding of nuclear fuels and material performance in the nuclear environment, at the nanoscale and lower, is critical to the development of innovative fuels and materials required for tomorrow's nuclear energy systems.*" [2]

Developing an advanced postirradiation examination (PIE) capability is very important to advance nuclear energy as an option to meet national energy goals. Understanding the behavior of fuels and materials in a nuclear reactor irradiation environment is the limiting factor in nuclear plant safety, longevity, efficiency, and economics. A state-of-the art PIE capability is required to transition into a "science-based" approach in the development of advanced fuels and materials, enabling a fundamental understanding of fuels and materials behavior under irradiation.

A National Postirradiation Examination (PIE) Workshop was held March 29-30, 2011, in Gaithersburg, MD, to identify the nation's needs for PIE to support advanced fuels and nuclear material development. It is part of broader goal to address the Department of Energy (DOE) missions in nuclear plant efficiency, economics, and safety, improved use of nuclear fuels, and fuel resources safe and publically acceptable solution to used fuel long-term storage and disposal, and reduced environmental impact of nuclear energy production and use.

During the workshop, the National PIE needs were identified from various perspectives, including universities, industry, vendors, Nuclear Regulatory Commission (NRC), Advanced Test Reactor (ATR) National Scientific User Facility (NSUF), and DOE Nuclear Energy (NE) national laboratories. Achieving the state-of-the art capabilities that can support a complete transition to science-based approach requires progressive set of actions:

The first step, after multiple decades of neglect, is to update and refurbish the existing capabilities and replace the older capabilities with newer, more accurate, and more reliable set of instruments.

The second step is to introduce advanced instruments and scientific techniques, commonly used in other applications with nonradioactive materials, into PIE applications. The objective is to start characterizing

2011
State of the Union Address
President Barack Obama

"This is our generation's Sputnik moment. Two years ago, I said that we needed to reach a level of research and development we haven't seen since the height of the Space Race…We'll invest in biomedical research, information technology, and especially clean energy technology…

That's what Americans have done for over 200 years: reinvented ourselves. And to spur on more success…we've begun to reinvent our energy policy… We're issuing a challenge. We're telling America's scientists and engineers that if they assemble teams of the best minds in their fields, and focus on the hardest problems in clean energy, we'll fund the Apollo projects of our time…

Now clean energy breakthroughs will only translate into clean energy jobs if businesses know there will be a market for what they're selling. So tonight, I challenge you to join me in setting a new goal: By 2035, 80 percent of America's electricity will come from clean energy sources.

Some folks want wind and solar. Others want nuclear, clean coal and natural gas. To meet this goal we will need them all – and I urge Democrats and Republicans to work together to make it happen." [1]

radioactive samples at nano-scale to micro-scale length resolutions. Some of these instruments, when applied to radioactive materials characterization, require special facilities with very strict environmental control.

The third step is to design and develop instruments that currently do not exist but are required to measure properties at various length and time scales in order to support a complete fundamental understanding of radioactive materials behavior. Such instruments would be valuable to understand separate effect phenomenology and to support the multi-physics, multi-scale, predictive fuel performance modeling efforts. These capabilities are also likely to require new facilities with very specialized environmental control and integration among multiple techniques.

During the workshop, breakout sessions were organized around the following topic areas:

- Fuel Cycle Research and Development/Fast Reactor Fuels
- Light Water Reactor Fuels
- Gas Cooled Reactor/Particle Fuels
- Modeling and Simulation/Scientific Measurements
- Nuclear Materials.

At the conclusion of the workshop, four high-level needs were identified as common themes from the five breakout teams. Those needs are summarized below:

1. Understanding material changes in the extreme nuclear environment at the nanoscale, especially for highly activated fuels and materials. Nanoscale studies have significant importance due to the mechanisms that cause materials to degrade, which occur at the nanoscale.
2. Enabling additional proficiency in experimentation and analysis through robust modeling and simulation coupled with advanced characterization.
3. Advancing the infrastructure and accessibility of physical and administrative systems to meet the needs of participating organizations. The inability to accommodate different time cycles and constraints make working and collaborating within the national laboratories challenging. This also includes the development of talent and the retention of expertise to support the research needs of the future.
4. Pursuing in-situ instrumentation and measurements to better examine dynamic changes to materials' microstructure, deformation, and surface effects as they occur in real time rather than the static, end-state data obtained by most current PIE methods. Also the ability to interpret the PIE data accurately requires a detailed understanding of the irradiation history and associated initial and boundary conditions.

The National PIE Workshop was also a response to the research challenges for advanced PIE needs for nuclear fuels and materials development outlined by Energy Secretary Chu and the *DOE-NE Research and Development Roadmap*, which was delivered to Congress in April 2010 [3]. PIE technial needs for nuclear fuels and materials development were identified for short-term (less than 10 years) and long-term (greater than 10 years) research. Gaps in existing PIE capabilities were discussed along with potential future solutions.

The National PIE Workshop Report will inform the identification and evaluation of alternatives in support of the CD-1 activities for state-of-the art PIE capabilities. It will also be used to support PIE strategic planning, define future capability needs, and support the conceptual designs for advanced PIE facility(ies) and associated instrumentation. For information regarding this report, please contact Kemal Pasamehmetoglu, National Technical Director for the Fuel Cycle R&D Advanced Fuels Campaign, at kemal.pasamehmetoglu@inl.gov.

CONTENTS

FIGURES

ACRONYMS

μ	micro
AES	Auger Electron Spectroscopy
AFM	Atomic Force Microscopy
AGR	Advanced Gas Reactor
AHTR	Advanced High Temperature Reactor
ANL	Argonne National Laboratory
ATR-NSUF	Advanced Test Reactor-National Scientific User Facility
BESAC	Basic Energy Sciences Advisory Committee
CO	Carbon Monoxide
DBTT	Ductile-Brittle Transition Temperature
DOE	U.S. Department of Energy
DPA	Displacements per atom
EDM	Electrical Discharge Machining
EDS	Energy Dispersive Spectroscopy
EELS	Electron Energy Loss Spectroscopy
EMI	electromagnetic interference
EPMA	Electron Probe Micro Analyzer
EPRI	Electric Power Research Institute
FCRD	Fuel Cycle Research and Development
FG	fission gases
FHR	Fluoride Salt-cooled High Temperature Reactor
FIB	Focused Ion Beam
FP	fission products
GCR	Gas Cooled Reactor
GNF	Global Nuclear Fuel
HR-TEM	High Resolution Transmission Electron Microscope
HTGR	High Temperature Gas Cooled Reactor
HTR	High Temperature Reactor
HTTR	High Temperature Test Reactor
IASCC	Irradiation Assisted Stress Corrosion Cracking
ICP-MS	Inductively Coupled Plasma Mass Spectrometry
IMCL	Irradiated Materials Characterization Laboratory
INL	Idaho National Laboratory
IVEM	Intermediate Voltage Electron Microscope

LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
LOCA	Loss-of-Coolant Accident
LWR	Light Water Reactor
M&S	Modeling and Simulation
MaRIE	Matter-Radiation Interactions in Extremes (LANL)
NDE	Non-destructive Examination
NE	Department of Energy Office of Nuclear Energy
NGNP	Next Generation Nuclear Plant
NRC	Nuclear Regulatory Commission
NRF	Nuclear Resonance Fluorescence
O/M	operations and maintenance
OIM	Orientation Imaging Microscopy
ORNL	Oak Ridge National Laboratory
PBR	Pebble Bed Reactor
PDF	atomic pair distribution function
PIE	Postirradiation Examination
PMR	Prismatic Modular Reactor
PNNL	Pacific Northwest National Laboratory
R&D	Research and Development
SANS	Single Angle Neutron Scattering
SAXS	Single Angle X-ray Scattering
SCC	Stress Corrosion Cracking
SEM	Scanning Electron Microscope
SiC	Silicon Carbide
SIMS	Secondary Ion Mass Spectrometry
SNL	Sandia National Laboratory
STDM	Statistical Time Division Multiplexing
STEM	Scanning Transmission Electron Microscope
TAMU	Texas A&M University
TEM	Transmission Electron Microscope
TRISO	Tristructural-Isotopic Fuel
XAS	X-ray Absorption Spectroscopy
XPS	X-ray Photoelectron Spectroscopy
XRD	X-ray Diffraction

National Postirradiation Examination Workshop

1. INTRODUCTION

The coupled challenges of a doubling of the world's energy needs by the year 2050 and increasing demands for "clean" energy sources that do not add more carbon dioxide and pollutants to the environment have resulted in increased worldwide attention to the possibilities of advanced nuclear energy as a long-term solution for a secure energy future. These two challenges were the focus of the Basic Energy Sciences Advisory Committee (BESAC) Subpanel Study, published in February 2003.[4] This report together with President Barack Obama's challenge to have 80 percent of America's electricity generation from clean energy sources by 2035 [1], supports a more detailed study of the basic research needs for nuclear energy.

On January 31, 2011, Peter B. Lyons, Acting Assistant Secretary for Nuclear Energy, approved Critical Decision (CD)-0, Approve Mission Need, for the Advanced Postirradiation Capability Project. As stated in the Mission Need, "*A better understanding of nuclear fuels and material performance in the nuclear environment, at the nanoscale and lower, is critical to the development of innovative fuels and materials required for tomorrow's nuclear energy systems."* [2] The National workshop and the resulting report is a partial response to the approval of the mission need for the Advanced Postirradiation Examination Capability project.

The needs for performing advanced postirradiation examinations (PIE) on highly activated nuclear fuels and materials is not new and has been debated by various panels and well documented in previous reports with a primarily scientific perspective. Several of these reports are excerpted in this document. In contrast to those reports, the current report generated through a workshop, provides a set of practical and application-focused recommendations in support of the activities to achieve critical decision 1 (CD-1) for the Advanced Postirradiation Examination Capability project.

1.1 The Role of Basic Science

The enormous gap between our present capabilities for nuclear energy production and use and those required to enable a sustainable and economically viable energy future was evident from the BESAC *New Science for a Secure and Sustainable Energy Future* [5] report, which states:

> *"These new advanced energy technologies however, require new materials and control of chemical change that operate at dramatically higher levels of functionality and performance…operating…nuclear power plants at far higher temperatures and efficiencies requires materials with atom by atom design and control, tailored nanoscale structure where every atom has a specific function. Such high performing materials would have complexity far higher than today's energy materials…*
>
> *"Creating these advanced materials and chemical processes requires characterizing the structure and dynamics of matter at levels beyond our present reach. The physical and chemical phenomena that capture, store, and release energy take place at the nanoscale, often involving subtle changes in single electrons or atoms, on timescales faster than we can now resolve. Penetrating [these] secrets of energy…requires new observational tools capable of probing the still-hidden realms of the ultrasmall and ultrafast. Observing the dynamics of energy flow in…systems at these resolutions is necessary if we are to learn to control their behavior."*

The report from the Office of Basic Energy Sciences workshop on *Basic Research Needs for Advanced Nuclear Energy Systems*, further clarified the need for materials research to address the challenges of the extreme environment in nuclear reactors.

"In addition, the effective utilization of nuclear power will require continued improvements in nuclear technology, particularly related to safety and efficiency. In all of these areas, the performance of materials and chemical processes under extreme conditions is a limiting factor. The related basic research challenges represent some of the most demanding tests of our fundamental understanding of materials science and chemistry, and they provide significant opportunities for advancing basic science with broad impacts for nuclear reactor materials, fuels, waste forms, and separations techniques. Of particular importance is the role that new nanoscale characterization and computational tools can play in addressing these challenges. These tools, which include DOE synchrotron X-ray sources, neutron sources, nanoscale science research centers, and supercomputers, offer the opportunity to transform and accelerate the fundamental materials and chemical sciences that underpin technology development for advanced nuclear energy systems.

"The fundamental challenge is to understand and control chemical and physical phenomena in multi-component systems from femto-seconds to millennia, at temperatures to 1000ºC, and for radiation doses to hundreds of displacements per atom (dpa). This is a scientific challenge of enormous proportions, with broad implications in the materials science and chemistry of complex systems. New understanding is required for microstructural evolution and phase stability under relevant chemical and physical conditions, chemistry and structural evolution at interfaces, chemical behavior of actinide and fission-product solutions, and nuclear and thermo-mechanical phenomena in fuels and waste forms." [7]

The basic research efforts called for by these reports, essentially nanoscale materials characterization on materials subjected to extreme radiation environments, is the basis for resolving many of the DOE Office of Nuclear Energy (NE) Roadmap challenges to increase the use of nuclear energy, domestically and internationally [3].

- The capital cost of new large plants is high and can challenge the ability of electric utilities to deploy new nuclear power plants.
- The exemplary safety performance of the U.S. nuclear industry over the past thirty years must be maintained by an expanding reactor fleet.
- There is currently no integrated and permanent solution to high-level nuclear waste management.
- International expansion of the use of nuclear energy raises concerns about the proliferation of nuclear weapons stemming from potential access to special nuclear materials and technologies.

"Resolving these challenges goes far beyond incremental advances in the present state of the art. Rather, fundamental breakthroughs are needed in the understanding and control of materials at the nanoscale. To be economically competitive with the present fossil fuel economy, the current fleet of reactors must have their life spans extended beyond 60 years, cost of new reactors must decrease by several factors, and fuels must become more sustainable and proliferation resistant. [3]

Historically, research on materials for nuclear environments has been conducted using extensive integral effects testing followed by primarily macroscopic characterization. Significant advances have been completed using this approach. However, other high technology industries have been successful using advanced instrumentation and techniques that allow research at the microstructure and nanoscale and then coupling these tools with the predictive capabilities of detailed modeling and simulation. These advanced tools have been used successfully across industries both nationally and internationally to improve material performance in extreme environments. Also, the capability to use multi-physics, multi-scale modeling and simulation to predict the fuel performance requires quantification of parameters that was not previously needed before in a purely empirical approach for fuels and materials development and qualification. Such instruments and measurement techniques must be developed and used in specialized facilities. Future applications of advanced instrumentation, PIE, and simulation techniques will be a major factor in all areas of nuclear energy research and application.

1.2 Current State of PIE Capability in the United States

The behavior of fuels and materials in a nuclear reactor environment is extremely complex and represents the limiting factor in plant safety, longevity, efficiency, and economics. Universities and DOE National Laboratories perform much of the basic science and research for the advancement of nuclear related materials and fuels. They currently provide the basic characterization and PIE functions, but are unable to test fuel and material behavior across micro, nano, and atomic scales, necessary for development and validation of time-resolved computer models of fuel and material behavior. The use of unique analytical instruments and technology on highly radioactive fuels and materials is a capability that has been nearly lost in the U.S.

Typically, they conduct exams in existing hot cell and radiochemistry facilities that are 30-50 years old and not designed to house modern research tools and instruments sensitive to vibration, electrical and magnetic fields, and temperature fluctuations.

The nation's nuclear research capability has been minimal the last 15 years and access to cutting-edge tools for research in nuclear sciences, technology, fuels, and materials is currently severely limited.

Advanced PIE capability is crucial for the United States to maintain and further a global leadership role in advancing safe and secure nuclear energy technology. Understanding nuclear fuel and material performance in the nuclear environment at the nano-scale is critical to the development of innovative fuels and materials for tomorrow's nuclear energy systems.

The DOE Office of Nuclear Energy (NE) mission will be difficult to achieve without establishing the capability to do research on highly radioactive fuels and materials.

With advanced PIE capability, the U.S. will maintain a global leadership role in advancing safe and secure nuclear energy technology. It will promote the development of nuclear research capability at the nano and sub-angstrom scales (10^{-9} to 10^{-10} meters). As a result, these capabilities can be made available to the broader nuclear energy research community as a user facility. Industry, universities, as well as DOE national laboratories will be able to grow and harness the intellectual capital of the country to advance U.S. R&D goals and objectives.

The Critical Decision (CD) 0 approval of the "Advanced Postirradiation Examination Capability" Mission Need Document on January 31, 2011, launched a national movement toward revolutionary improvements in our nuclear fuels and materials research capabilities. The PIE Workshop was organized to support the next step in the critical decision (CD-1) process by identifying PIE needs at a national level across a broad user community. Identifying the capability (facilities, equipment, and expertise) to meet the needs is the next step. We may find gaps in our national infrastructure that will need to be filled to meet DOE's future nuclear energy goals. In implementing the PIE capabilities project, there are three major steps:

The first step, after multiple decades of neglect, is to update and refurbish the existing capabilities and replace the older capabilities with newer, more accurate, and more reliable set of instruments.

The second step is to introduce advanced instruments and scientific techniques, commonly used in other applications with nonradioactive materials, into PIE applications. The objective is to start characterizing radioactive samples at nano-scale to micro-scale length resolutions. Some of these instruments, when applied to radioactive materials characterization, require special facilities with very strict environmental control.

The third step is to design and develop instruments that currently do not exist but are required to measure properties at various length and time scales in order to support a complete fundamental understanding of radioactive materials behavior. Such instruments would be valuable to understand separate effect phenomenology and to support the multi-physics, multi-scale, predictive fuel performance modeling efforts. These capabilities are also likely to require new facilities with very specialized environmental control and integration among multiple techniques.

2. WORKSHOP OVERVIEW

The National PIE Workshop had approximately 55 representatives from universities, industry, vendors, DOE national laboratories, DOE Headquarters, and Nuclear Regulatory Commission (NRC). Opening remarks were provided by Dennis Miotla, Deputy Assistant Secretary for Nuclear Facility Operations. He discussed the two primary objectives of his office, which is to:

- Ensure that the DOE-NE R&D Programs have the facilities they need to accomplish their work.
- Ensure that facilities are acquired, operated, maintained and disposed of in a safe, secure, reliable and efficient manner.

> ***DOE-NE Mission***
> *Advance nuclear power as a resource capable of meeting the Nation's energy, environmental, and national security needs by resolving technical, cost, safety, proliferation resistance, and security barriers through research, development, and demonstration as appropriate. [3]*

Kemal Pasamehmetoglu, National Technical Director for Advanced Fuels Campaign in the DOE-NE Fuel Cycle Research and Development Program, discussed the purpose of the workshop, which was organized to solicit input (needs) from the technical community to develop state-of-the art characterization and PIE capabilities in support of nuclear fuels and materials development. Representatives from the technical community, industry, vendors, universities, and DOE national laboratories, were invited to present their PIE and Characterization needs from a variety of perspectives. A video was shown to highlight the U.S. need for advanced PIE capability as well as the current gaps in technology. Breakout sessions were organized to provide the opportunity to collect individual and group technical PIE needs, opportunities, and barriers. This information was presented by the session leads at the conclusion of the workshop.

2.1 DOE-NE R&D Roadmap Objectives Rely on Advanced Research

Dennis Miotla emphasized the commitment by DOE-NE to build a strong nuclear energy program in the U.S. The following are the DOE-NE Mission Level Assumptions that drove the creation of the *DOE-NE Research and Development (R&D) Roadmap* [3] and associated four objectives (see Figure 1):[2]

- *The United States must develop and deploy clean, affordable, domestic energy sources as quickly as possible to achieve energy security and greenhouse gas emission reduction objectives .*
- *Nuclear power will continue to grow as a key component of a portfolio of technologies that meets the nation's energy goals.*
- *DOE-NE will resolve technical, cost, safety, security, and regulatory challenges through science-based and applied programs in the development of advanced nuclear fuels and materials.*
- *U.S. commercial nuclear power industry will pursue development of nuclear fuels and materials with enhanced reliability, increased performance, enhanced accident tolerance and reduced waste production in partnership with DOE-NE.*

Advanced modeling and simulation can lead to new theoretical understanding and, in turn, can improve models and experimental design. This R&D must be informed by the basic research capabilities in the DOE Office of Science (SC).

NE maintains access to a broad range of facilities to support its research activities, such as hot cells, test reactors, radiological facilities, specialty engineering facilities, and small non-radiological laboratories. NE employs a multi-pronged approach to having these capabilities available when needed. The core capabilities rely on DOE-owned irradiation, examination, chemical processing, and waste form development facilities. These are supplemented by university capabilities ranging from research reactors to materials science laboratories. In the course of conducting this science-based R&D, infrastructure needs will be evaluated and considered through the established planning and budget development processes.

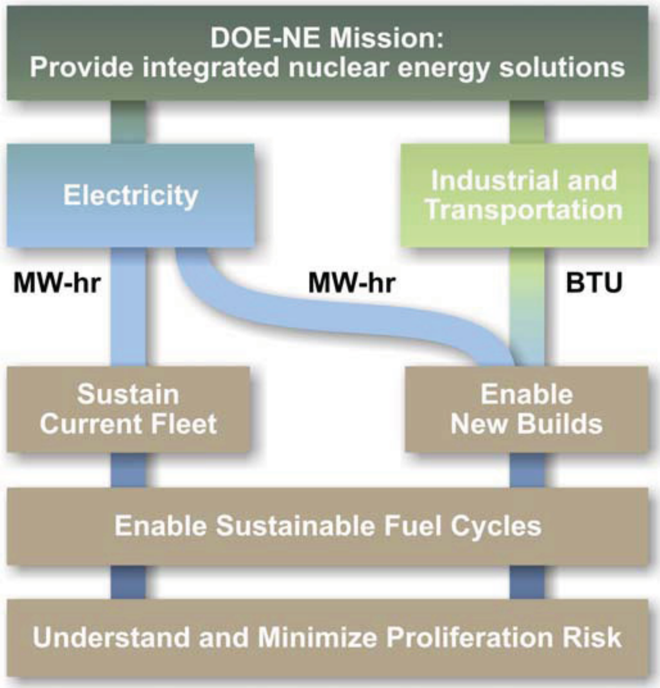


Figure 1: DOE-NE R&D Mission Roadmap

2.2 Goal Oriented, Science-Based Approach

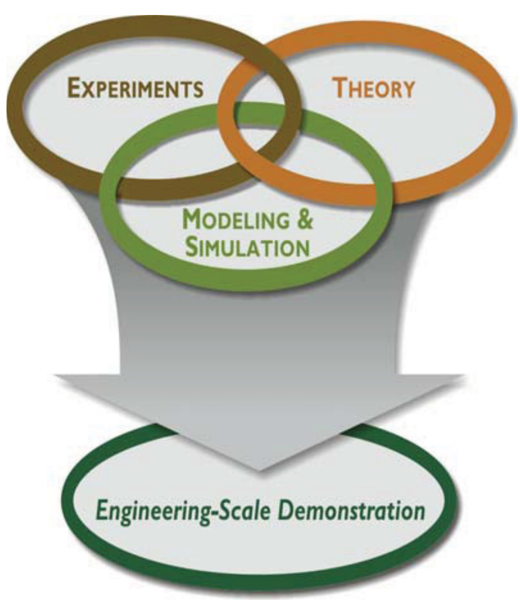


Figure 2: Major Elements of a Science-Based Approach

The DOE-NE R&D Roadmap outlines the "Goal Oriented Science-Based" approach, depicted in Figure 2. It combines theory, experimentation, and high-performance modeling and simulation to develop the fundamental understanding that will lead to new technologies. Advanced modeling and simulation tools will be used in conjunction with smaller-scale, phenomenon-specific experiments informed by theory to reduce the need for large, expensive integrated experiments. Insights gained by advanced modeling and simulation can lead to new theoretical understanding and, in turn, can improve models and experimental design.[3]

Applying this approach to nuclear fuels and materials development requires an iterative process involving fuel fabrication, characterization, irradiation testing, PIE, and back to fuel fabrication. See Figure 3 to see how the process flows and interacts with modeling and simulation.

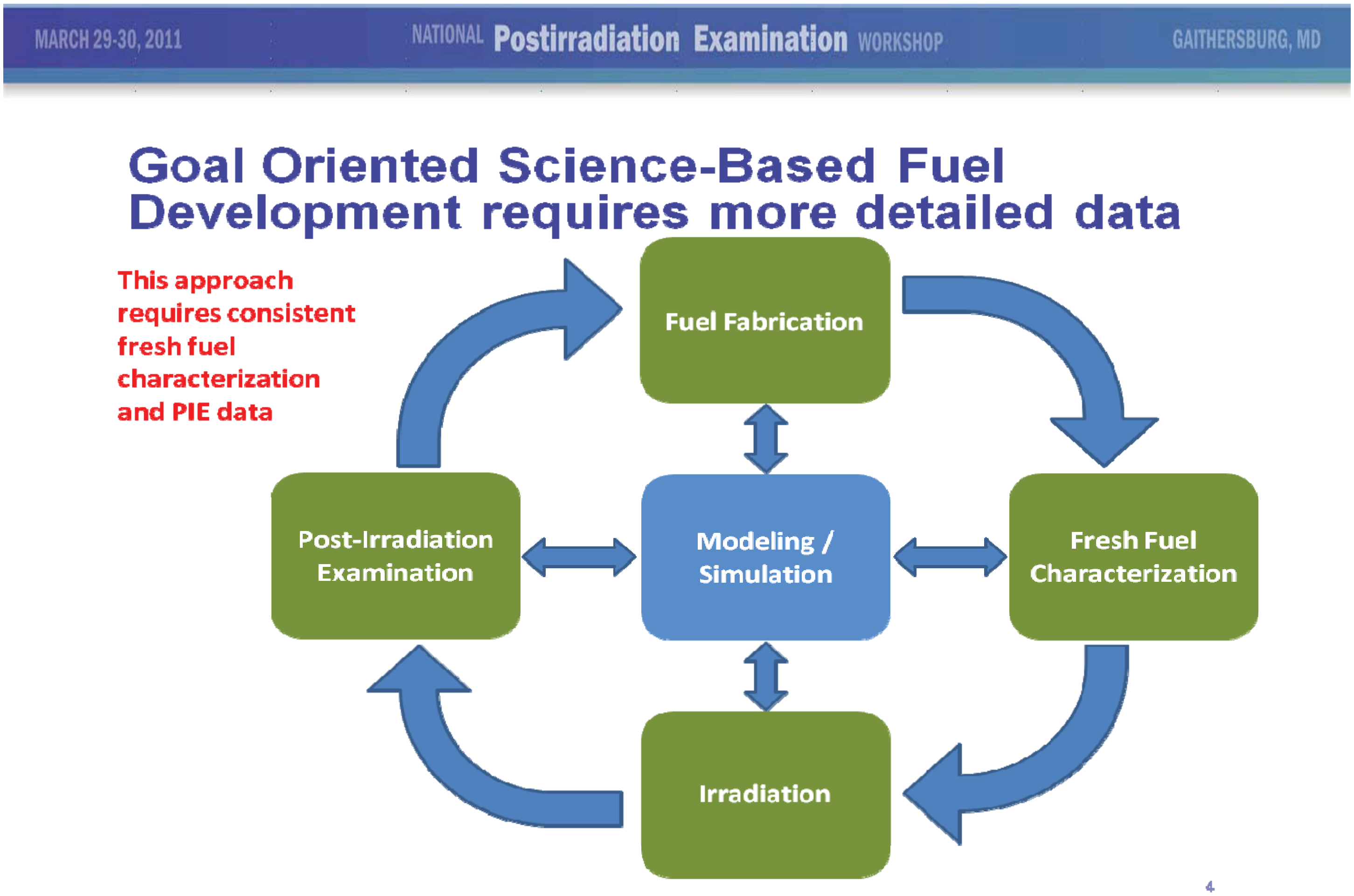


Figure 3: Goal Oriented Science-Based Fuel Development

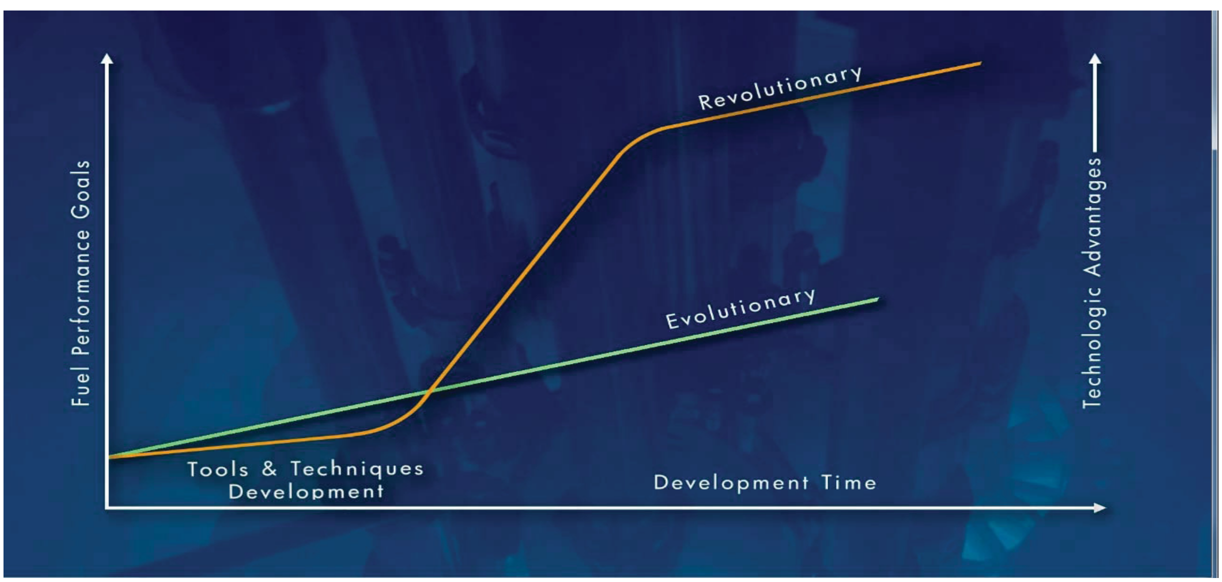


Figure 4: Revolutionary Fuel and Material Development

The coupling of focused phenomenological testing, theory development and modeling and simulation techniques advances nuclear fuel development from evolutionary to revolutionary. Embarking into a revolutionary fuels and materials development paradigm originally requires an incubation period, during which the intellectual and hardware infrastructure is implemented. However, once the infrastructure is in place. Figure 4 shows how advanced tools and techniques optimizes development time and significantly improves the technologic advantages in reaching higher fuel performance. The U.S. needs to move from empirical correlations to describe fuels and materials behavior under irradiation and to understanding and predicting the changes in material microstructure that give rise to these behaviors. We need to develop the capability to predict the evolution of microstructure of fuels and materials under irradiation, and from that microstructure infer materials properties and performance. The coupling of these correlations with advanced modeling and simulation across length scales from the nano- to engineering-scale is critical to achieving nuclear energy goals at an accelerated pace (see Figure 5).

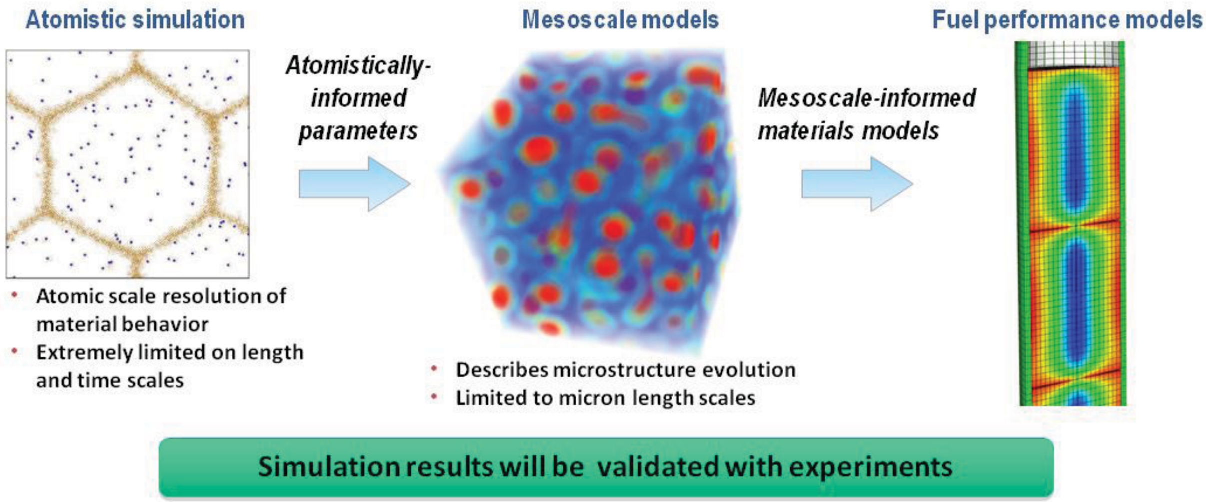


Figure 5: Advanced Modeling and Simulation requires higher fidelity data at lower length and time scales.

2.3 U.S. Perspectives on PIE and Characterization Needs

Technical presentations were provided to broadly represent national PIE needs from university, industry, vendor, user facility, NRC, and national laboratory perspectives. This section contains a high level summary of the presentations, which were given by the following representatives:

- Industry Perspective, Energy Power Research Institute (EPRI), by Kemal Pasamehmetoglu, INL
- Vendor Perspective, Current and Future Needs for PIE, by Michael Burke, Westinghouse Electric Company LLC
- DOE-NE Research, by Steven L. Hayes, Idaho National Laboratory (INL)
- University Fuel Research, by Sean M. McDeavitt, Texas A&M University (TAMU)
- Advanced Test Reactor (ATR) National Scientific User Facility (NSUF), by Todd Allen, University of Wisconsin
- PIE and Testing: A Regulatory Perspective, by John Voglewede, Nuclear Regulatory Commission (NRC)
- Used Nuclear Fuel Perspective, by Ruth Weiner, Sandia National Laboratory (SNL).

Industry. World-class hot cells, maintenance of basic PIE equipment, and PIE expertise are critical to quick turnaround of the data analysis. Industry also needs easy access to facilities, data, and analyses. Specifically they are interested in fuel failure root cause and testing with increased throughput at smaller scales. They must have sample disposal at the PIE facility, since they have no means to handle fuel and samples after destructive analysis.

Commercial Vendors. Support for fuel failure analyses is at the top of their priority list. They also need reactor pressure vessel and internals' materials degradation analyses, assessment of new fuel cladding alloys, and support for long-term plant and nuclear fuel related materials development. They need data from highly radioactive samples ranging from scrapings to bulk samples. They must have sample disposal at the PIE facility, since they have no means to handle fuel and samples after destructive analysis.

DOE-NE Research. One of the fuels research goals is to develop improved science-based materials models for fuel performance using hierarchical multiscale modeling. Macroscopic (standard NDE and DE) and micro-/nano-scale characterization of irradiated fuels and materials are needed to inform the modeling and simulation effort.

University Research. Access to DOE national laboratory facilities and inclusion in major research programs are two critical needs for students and professors. They want to be the "users" and "developers" of PIE capabilities with access to state-of-art infrastructure within the national laboratory system. Universities have timing issues when working with long-term research projects, such as fuel and material development, which can take up to 30 years, considering the student cycle is 2-3 years and the DOE funding cycle is yearly. Therefore, they need short turnaround publications and theses and involvement in major, longer-term DOE programs.

National Scientific User Facilities. ATR-NSUF needs access to test reactor space and existing PIE capability. Users need modern microscopes, surface science capability, electrochemical capability and nano-scale mechanical testing. The critical infrastructure needs to be in place for sample preparation, radioactive sample analysis, and irradiation testing from various sources. In the near future, users will need access to a broad range of instruments and testing facilities as well as in-situ instrumentation to validate PIE data.

Nuclear Regulatory Commission. Fuel, cladding, and component performance under accident conditions is more important than in steady-state operation. Additional characterization (e.g., microchemistry, microstructure, etc.) is needed for these off-normal conditions for both irradiated and unirradiated materials. The NRC assumes that PIE facilities will have the following abilities:

- To handle, non-destructively examine, disassemble, and section full-length assemblies and rods.
- To resolve short-term and long-term ownership issues for irradiated fuel and cladding materials.
- To archive irradiated fuel and cladding materials for follow-up studies.
- To handle long-term disposal issues.

The NRC has never before licensed a nuclear reactor fuel based solely on computer model predicted behavior, and is unlikely to do so before enhanced modeling capability has been validated through physical testing [and post-irradiation examination]. [13]

Used Fuel Storage. PIE capability is needed to analyze issues related to long-term storage of nuclear fuels and materials. Analysis on increasingly smaller-length scales is required to understand the phenomena that cause material degradation during long-term storage. PIE capabilities for used fuel include the following:

- Elevated temperature testing of fueled and unfueled rod lengths for fatigue, pressurized capsule testing, mechanical properties (fracture toughness, yield, tensile) testing
- Metallography and ceramography of fueled samples
- Fission gas puncturing for fission gas release and void volume
- Fuel particulate sizing capabilities 3mm to .01 microns
- Profilometry on rods and rod segments
- Gamma scans capabilities on rods and rod segment
- Receive and handle whole rods, whole assemblies
- Long segment rodlet defueling capabilities
- Eddy current, ultrasonic testing of rods and rodlets.

2.4 Irradiated Materials Characterization Laboratory (IMCL)

As a first step to implementing the advanced PIE capabilities, the U.S. Department of Energy has initiated the design of a small facility, the IMCL at the Idaho National Laboratory. The IMCL (see Figure 6) will be the first facility of its type in the United States designed specifically for advanced instrumentation and equipment. The IMCL will contain space for installation of instruments and equipment within shielding structures that can be redesigned and refitted whenever necessary. The IMCL will also have mechanical systems that tightly control temperature, electrical and magnetic noise, and vibration to the standards required for advanced analytical equipment. Although some of the advanced characterization equipment is already in use in other industries, IMCL will be unique in the United States because the equipment will be housed in a nuclear facility and dedicated to the examination of irradiated fuels and materials.

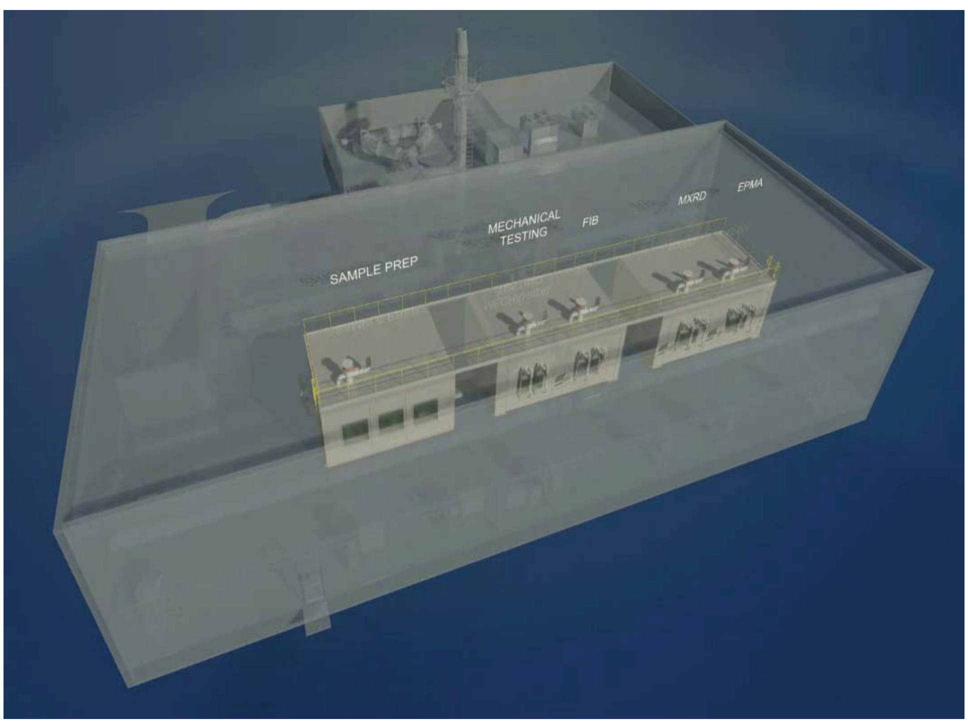


Figure 6: IMCL Layout

Designed as a multipurpose facility suitable for many different missions over its projected 40-year life, the IMCL will have as its first mission the task of housing modern, state-of-the-art PIE instrumentation. The IMCL will be used to routinely perform micro- and nano-scale characterization of material specimens and irradiated fuel samples in the mass range of tens of grams down to micro-grams. The facility will also be designed to allow easy routine maintenance of the instruments. The initial suite of equipment planned for installation into IMCL includes (see Figure 7):

a) Electron Probe Micro Analyzer (EPMA)

b) Focused Ion Beam (FIB)

c) Micro-X-ray Diffractometer (MXRD)

d) Field Effect Gun-Scanning Transmission Electron Microscope (FEG-STEM)

e) Mechanical Testing

f) Sample Preparation.

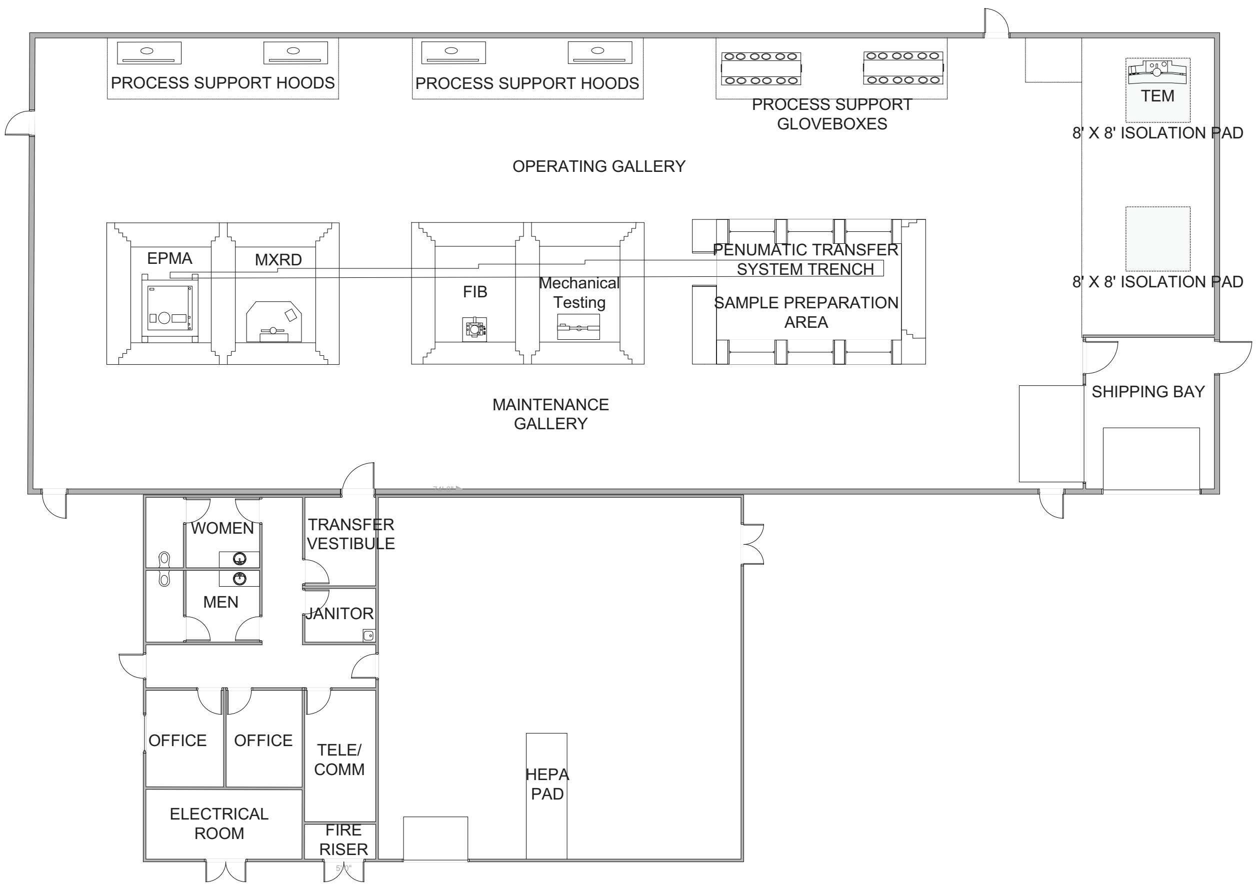


Figure 7: IMCL Conceptual Floor Plan

2.5 Technical Breakout Sessions

Workshop participants were divided into breakout teams to represent five technical categories. They were tasked to identify PIE and characterization needs in both the short-term (less than 10 years) and long-term (greater than 10 years). Discussion questions were provided to capture "what" is needed, "why" it is important, "how" the need could be met, and the gaps to meeting the need. Below are the technical categories and session chairs, along with the discussion questions:

- Fuel Cycle R&D (FCRD)/Fast Reactor Fuel – Ken McClellan, PhD, LANL
- Light Water Reactor – Todd Allen, PhD, University of Wisconsin
- Gas Cooled Reactor/Particle Fuels – Lance Snead, PhD, ORNL
- Modeling and Simulation/Scientific Measurements – Steve Hayes, PhD, INL
- Materials – Tarik Saleh, PhD, LANL

Focus questions for the breakout sessions:

- Technical Needs (What)
  - What do you want to measure, but don't know how today?
  - What advanced/enhanced capability is needed?
  - What are the accuracy and throughput requirements? Where are we now?
- Basis (Why)
  - Why is it important, why will it be important?
  - How will you use the data?
- Solution (How, Who, Where)
  - How can the need be met?
  - Where are existing capabilities? (Equipment, facilities, techniques, resources, etc.)
  - Can existing capabilities be modified?
- Gap (Barrier)
  - What capabilities are not available?
  - What capabilities need to be developed or invented?

PIE and characterization needs identified for accelerating nuclear energy innovation during the introductory presentations and during the breakout session are included in the subsequent sections and in the appendices.

Clearly, the discussions during a 2-day workshop cannot provide 100% coverage of all the needs, potential future innovations, implementation strategies, etc. The resulting report with responses to the above questions provides a practical overview of the current and desired future landscape. As we proceed to implement the details, this report will be used in conjunction with the previously cited reports with broader scientific depth and similar International PIE capability assessments.

3. BREAKOUT SESSIONS: CURRENT AND FUTURE NEEDS

Each breakout session was tasked to identify PIE and characterization needs for fuel and highly activated (nuclear) materials. Additional detail concerning the needs identified in this section can be found in the appendix. The first three breakout sessions on nuclear fuel development are included together in subsection 3.1, Advanced Fuels Development. Nuclear Materials is in Subsection 3.2 and Modeling and Simulation is in Subsection 3.3.

3.1 Advanced Fuels Development

> "Future-generation reactor systems will use advanced materials and fuels technologies to implement advanced designs. Moving beyond current light water reactor (LWR) technology will enable reactors to operate with improved efficiency and improved economics. Improved designs using advanced materials may reduce the capital costs associated with plant construction. Three prominent examples of advanced reactor technologies are:
>
> - Graphite moderated thermal-spectrum reactors, such as the Next Generation Nuclear Plant, that operate at high temperature for efficient generation of electricity and heat delivery for non-electric applications
> - Fast-spectrum reactors that provide options for future fuel cycle management and electricity generation
> - Small modular reactors that may provide capital cost and manufacturing advantages over current systems." [8]

The advanced fuels development needs identified in the three breakout sessions were similar so they were combined in this section.

3.1.1 Program Descriptions

Representing different fuel types, three different fuel development areas were discussed in the workshop. These were FCRD/Fast Reactor Fuel, Light Water Reactor Fuel, and Particle/High-Temperature Gas Cooled Reactor Fuel. Each of the programs has unique attributes and goals. A brief summary of each program is included as follows.

FCRD/Fast Reactor Fuel Program. The primary responsibility is to develop advanced fuel technologies using a goal-oriented, science-based approach. This approach requires a micro-structural understanding of a broad spectrum of nuclear fuels and cladding materials. The science-based approach enables a fundamental understanding of fuel and cladding performance by incorporating data from postirradiation characterization at the micro-and nano-scales into a suite of modern computer modeling and simulation tools.

The FCRD program is also responsible for developing interim disposition strategies for used nuclear fuel. There is a need to extend the allowable interim dry storage period for those fuels presently in storage up to 120 years. Additionally, as commercial utilities pursue higher burn-up fuels in existing reactors, those changes must be considered by the Nuclear Regulatory Commission (NRC) to allow storage licenses to be granted. Understanding the performance of fuel, clad, assembly component and cask materials degradation as a function of time and environment is essential for the development of the predictive models that will be used to consider long-term dry storage performance with confidence. A science-based approach to this work will reduce the cost and schedule requirements to obtain the data necessary to extend licensed interim dry storage. [2]

Light Water Reactor Fuels Program. There is a large environmental and economic benefit in extending current commercial nuclear plant lifetimes. The key issue facing life extension efforts for current reactors is the radiation-induced degradation of materials. Materials research provides an important foundation for managing the long-term operation of existing plants. Development of the scientific basis to allow the evolution of fuels, understanding and predicting long-term degradation behavior, and operational limits of materials relies on detailed PIE of reactor fuels and materials on the lower length scales (nanometers). This data is required to build accurate, predictive computational models useful for the prediction of reactor service life. [2]

Gas Cooled Reactor /Particle Fuels. The operating conditions for High Temperature Gas Cooled Reactors (HTGR) represent a major departure from existing water-cooled reactor technologies. Few choices exist for metallic alloys for use at HTGR conditions and the design lifetime considerations for the metallic components impact the maximum operating temperature. Qualification of materials for successful application at the high-temperature conditions and 60-year-design life planned for HTGRs is a large portion of the effort in the development program. [9]

Coated particle fuels tristructural-isotopic (TRISO) are being applied in production scale in the U.S. Advanced Gas Reactor (AGR) program, the Japanese High Temperature Test Reactor (HTTR) program, and the Chinese High Temperature Reactor (HTR)-10/HTR-PM Program. Basic TRISO fuel development is done in the NGNP program. R&D for the next generation application of coated particle fuels is ongoing under the FCRD program. Areas for which active and low-level activities are expected are shown in Figure 8.

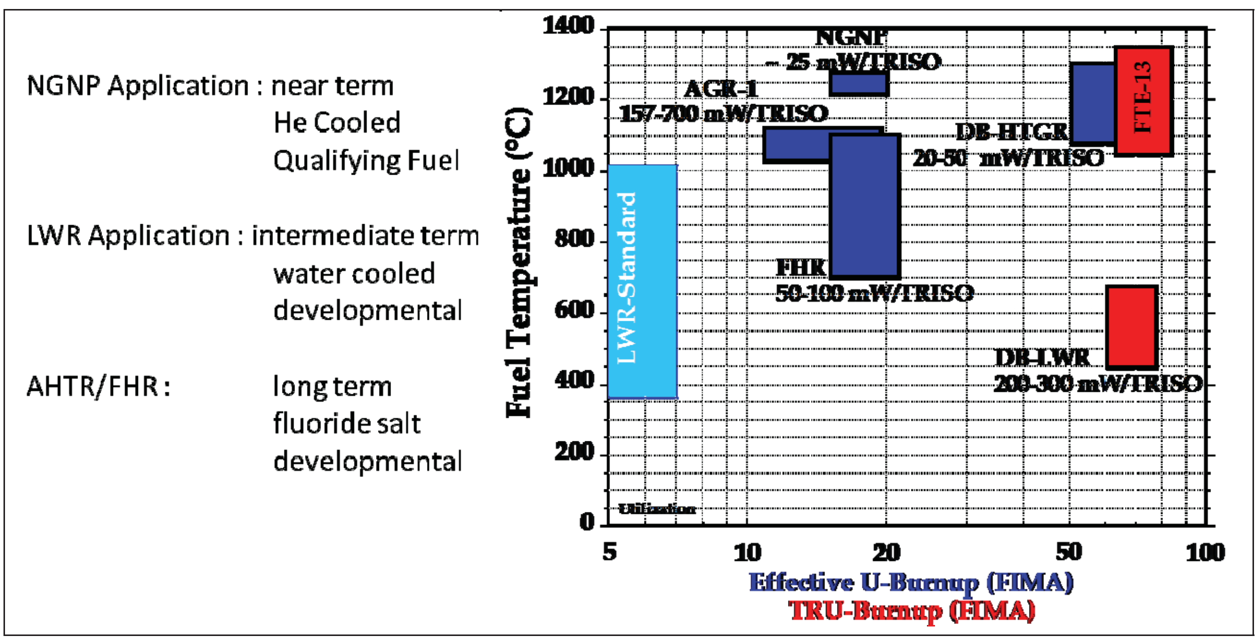


Figure 8: Coated Particle Fuel Activities

The objective of the DOE Advanced Gas Reactor (AGR) Fuel Development and Qualification program is to qualify TRISO-coated particle fuel (see Figure 9) for use in HTGRs. The NGNP/AGR Fuel Development and Qualification Program was established to provide a fuel qualification data set in support of the licensing and operation of the NGNP. Gas-cooled reactor fuel performance demonstration and qualification comprise the longest duration research and development task required for NGNP design and licensing. The fuel form is to be demonstrated and qualified for service conditions enveloping normal operation and accidents.[10]

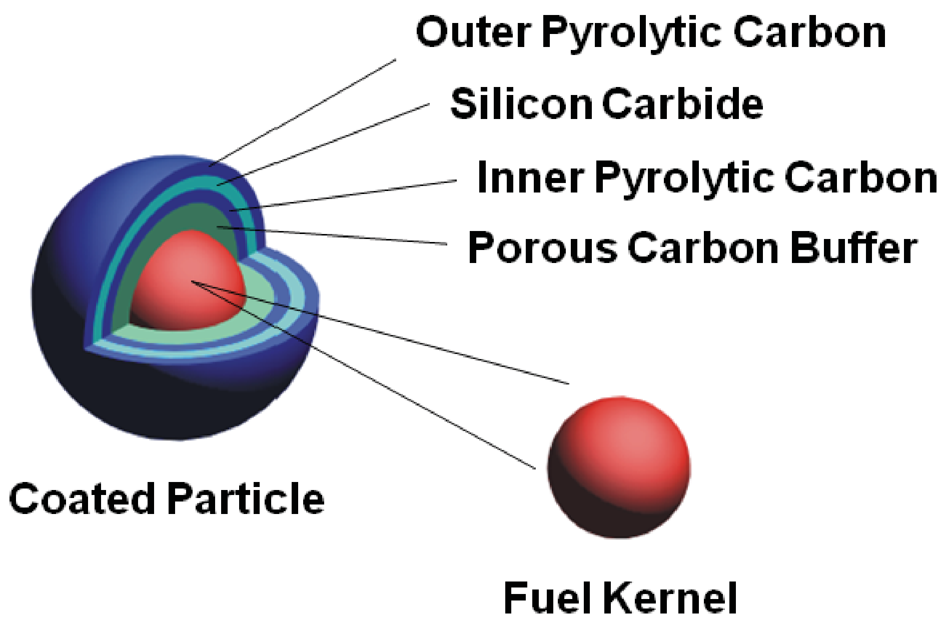


Figure 9: TRISO Fuel

3.1.2 Short-Term Advanced Fuels Development Needs

Several common high priority short-term needs were identified for these three distinct fuel development programs.

Detailed Microstructural and Thermal Properties Data: Examinations of the detailed microstructural and thermal properties data includes the need to evaluate fission product distributions (and associated local thermal properties), as well as hydride re-orientation and rim structure, because of the effect these have on corrosion and radiation effects in both fuel and cladding. These items also have significant effect on weld integrity and thermal conductivity.

Microstructural and Chemistry Data: Thermochemical evolution of fuel constituents is poorly understood and experimental definition is needed to baseline modeling efforts. The properties of pyrocarbons are unknown, and the SiC shell of TRISO fuel (the basis for TRISO fission product retention) needs to be understood. This includes investigations into the smaller spatial resolution of isotopic, composition, phase content and distribution, boundaries/interfaces, grain size and distribution, void distribution, and defects in fuel and cladding materials down to the ~10 nanometer scale.

Mechanical Properties Data: Mechanical properties data such as tensile strength and toughness, fatigue, and environmentally assisted fatigue, corrosion cracking (both stress and irradiation assisted), weld integrity, and flexion and vibration of large or full-size components is needed to predict safety of plant performance and also to support transportation and storage evaluations. Mechanical strength data is also specifically needed for TRISO particle fuels shell materials (see Figure 10) because of the need to understand the ultimate pressure capability for fission products and to provide information to benchmark modeling.

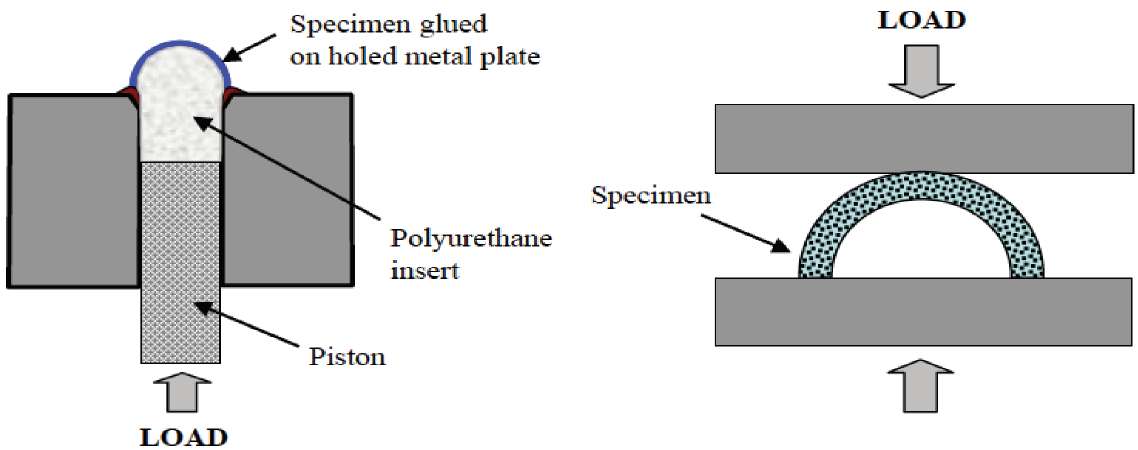


Figure 10: Strength Testing of Intact TRISO Fuel

***Logistics, Administration and* Infrastructure**: Logistics, administration and infrastructure is a significant area with many far reaching elements. The needs here include the ability to transport, receive, section, and analyze full length fuel rods; ability to receive, store, and section large components; and an administrative system that supports paying customers with on-time, on-budget project delivery. Some of the more specific needs in this category include improvements to the systems that produce, analyze, and dispose of PIE samples. This can include throughput, cost per sample, uniform, automated sample preparation, transportation, disposal, etc. These systems that need improvement can also include hot cells that need to be flexible or reconfigurable for different activities, the ability to isolate areas of cells, next generation removal operations and visualization for operators, very stringent environmental controls for factors such as atmosphere, temperature, purity, moisture, vibration, electromagnetic interference, etc. Cells for performing the needed work also need the ability to perform cask handling (small to large), be able to reconstitute pins/experiments, and handle both fuel and bond materials (sodium/lead, etc.). Also capabilities need to be configured to handle time sensitive examinations.

***Integral Measurements, Gross* Scale**: Despite the emerging need to perform PIE on smaller length and time scales, the need to perform irradiation testing of integral effects, with measurements at the engineering scale in order to assess assembly performance will continue.

Sample Library and Sample Analysis Support: A capability is needed to provide a sample library and sample analysis support including the storage of un-irradiated archive samples. This includes the quality assurance of samples to maintain pedigree, store, and manage data in a way that protects intellectual property but also makes data available to those interested, and finally includes a path for disposal of samples. This is important as re-analysis of samples can contribute significant value as measurement techniques improve, and reduces the need to re-perform costly irradiation of samples.

Remote Characterization: This is important for two reasons. First, to perform analysis in core for isotope assay, temperature distribution, location of rod breaches without pulling rods from assemblies, detection and location of nanoparticles from noble chemical additions or from burst testing, NDE of welds to improve technique, and as a precursor for finding flaws for further sectioning, isolation, and examination. The second reason is the need for remote installation of advanced characterization equipment to support analysis on higher activated materials.

The following are some specific needs identified for coated particle fuels, but the techniques would have a wider use.

Diffusion and Reactivity of Fission Products with SiC: The release of fission products is remains an unresolved issue. With specific reference to TRISO fuel, silver release and palladium attack are serious threats to TRISO breaches.

High Temperature Fuel Performance in Air/Steam: The evaluation of fuel performance under high temperature air and steam conditions is critical to acceptance and licensing.

Determine Internal TRISO Gas Pressure and Gas Species: The evolution of fission products and carbon monoxide (CO) within TRISO are needed as drivers for failure prediction and to benchmark modeling efforts.

***Measurement of High Temperature Iodine* Release**: Iodine is a most important contributor to offsite dose. Thus data is needed to determine the mechanisms and amount of high temperature iodine release.

Fission Product Distribution in Graphite: It is important to understand the fission product distribution, transport, and retention in graphite and how fission products affect graphite performance.

Environmental Testing with Non-Graphite Matrix: Alternative reactor platforms have non-standard matrices and require environmental and off-normal (e.g. LOCA) testing.

3.1.3 Long-Term Advanced Fuels Development Needs

In-Situ, Active, Real-time Monitoring of Evolution: The long term needs developed by the three fuel technology groups fundamentally mirror the short-term needs with the addition of continual modernization towards in-situ monitoring of fuel and material properties. Real-time in-situ monitoring of fuel and material changes as they occur is a valuable future capability as opposed to only being able to measure step changes from irradiated samples.

Advanced Non Destructive Examinations and Tomography: Advanced NDE is needed to target in-depth analysis more precisely (locating the place to cut and sample materials). It is also needed to measure clearly distinct fuel from cladding/structural material over the length of the disruptive zone. In addition, the ability to measure initial state and conditions before irradiation (steady and transient) is needed for comparison to postirradiation changes to density, chemical (elemental and isotopic), dimensions, and microstructure (see Figure 11).

Remote Robotics Manipulation: The ability to perform remote robotics manipulation of samples and sample preparation is needed to provide increased consistency for statistical analysis and reduce dose for performing analysis.

Test Assembly Corrosion (Salt, Water, Etc.) Loop for Irradiated Fuel Form: The next generation of advanced TRISO-bearing reactors could utilize fluoride salt, water, helium, etc as a coolant. Thus mass transport and corrosion will be issues at the sample, pin, and test assembly level. Tests will need to be carried out on irradiated fuel to examine these corrosion issues.

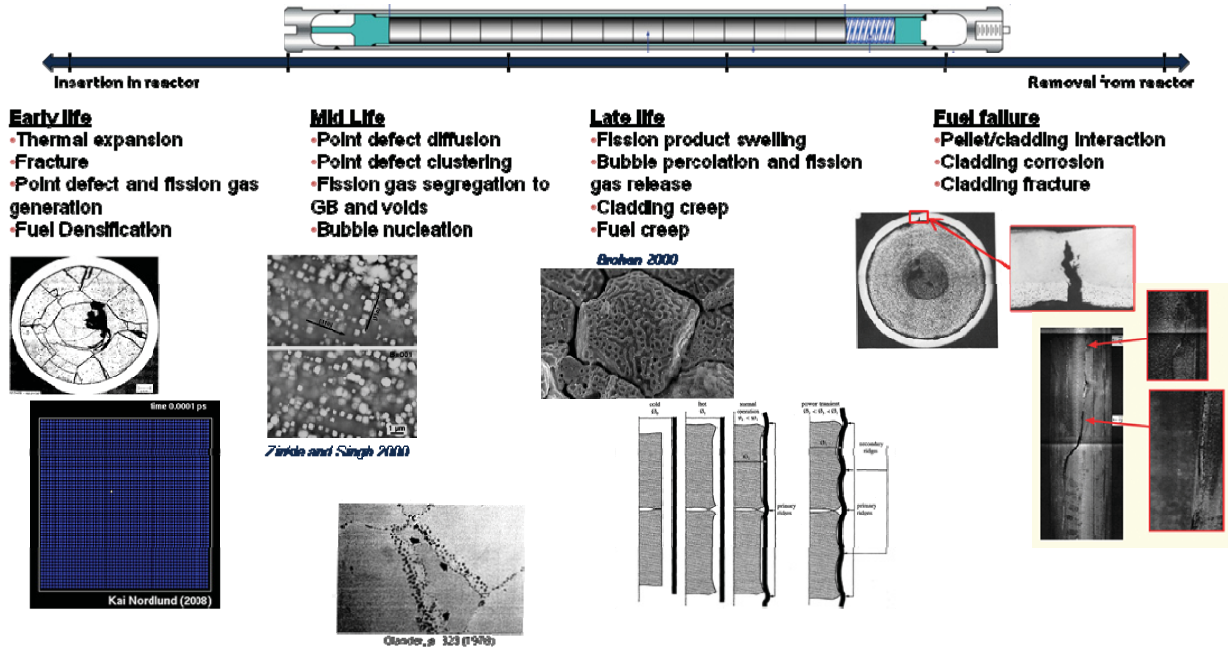


Figure 11: Microstructure Evolution in LWR Fuel

3.1.4 Conclusions

The FCRD Breakout Session concluded that more measurements are needed to evaluate chemistry, microstructure, properties, and integral measurements with spatial resolutions to be matched to these areas according to the need. Maintain engineering-scale measurements and increase access to smaller length and time scale measurements for fuel and cladding materials. Following this increase in measurement, access to the PIE data and support statistical analysis is needed with increased throughput and a lower cost per sample. Finally, develop techniques and capabilities that could perform technical measurements, but install as little equipment into hot cell configurations as possible by following a graded approach that includes using smaller sample sizes and shielding configurations in addition to hot cells.

The LWR Breakout Session concluded that their most important needs were detailed microstructural, thermal, and mechanical data obtained at smaller length and time scales than what is currently available for highly activated fuels and cladding materials. In addition, administrative structure (infrastructure) is needed to support paying customers with accessibility of both facilities and data. This includes handling full-length rods and providing sample libraries and sample analysis support. Meeting these needs would support attaining the goals for developing more robust models and increasing the lifespan of the current LWR fleet.

The GCR/PF Breakout Session concluded that the ability to perform micro-structural/micro-chemical analysis of highly irradiated material is needed, which would greatly enhance the future development of TRISO fuel. The data gathered from examinations at the micro-scale level could feed into a model that when validated would assist in the fuel development process. The proper infrastructure for doing these examinations is not currently in place.

3.2 Nuclear Materials

The Nuclear Materials Breakout Session identified their PIE and characterization needs in the short-term and long-term relative to materials development.

3.2.1 Nuclear Materials Development Description

Materials are central to every energy technology, and future energy technologies will place increasing demands on materials performance with respect to extremes in stress, strain, temperature, pressure, chemical reactivity, photon or radiation flux, and electric or magnetic fields. Next-generation nuclear fission reactors require materials capable of withstanding higher temperatures and higher radiation flux in highly corrosive environments for long periods of time without failure. These increasingly extreme operating environments accelerate the aging process in materials, leading to reduced performance and eventually to failure.

There are four recurring science issues for materials under extreme environments:

- Achieving the Limits of Performance
- Exploiting Extreme Environments for Materials Design and Synthesis
- Characterization on the Scale of Fundamental Interactions
- Predicting and Modeling Materials Performance.

Gaps in materials performance under extreme conditions could be bridged if the physical and chemical changes that occur in bulk materials and at the interface with the extreme environment could be understood from the atomic to macroscopic scale (see Figure 12). These complex and interrelated phenomena can be unraveled as advances are realized in characterization and computational tools. These advances will allow structural changes, including defects, to be observed in real time and then modeled so the response of materials can be predicted. The knowledge needed to bridge technology gaps requires significant investment in basic research, coupled closely with the applied research and industrial communities that will drive future energy technologies.[6]

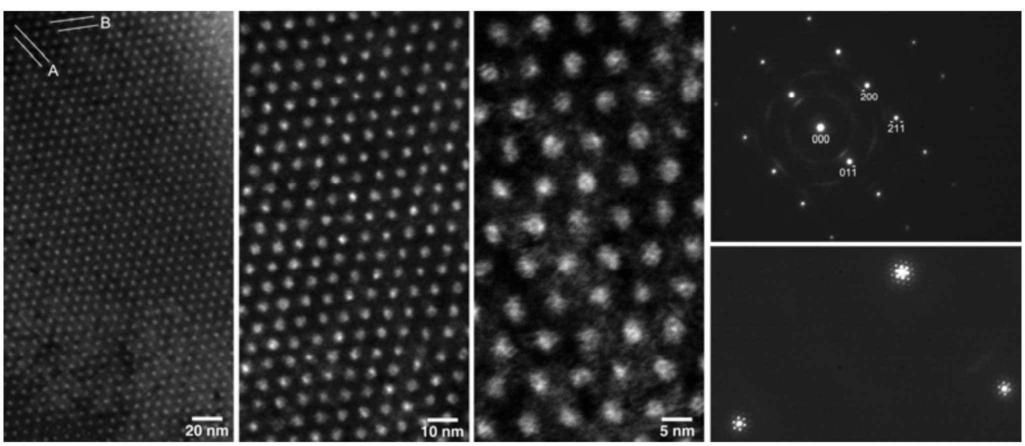


Figure 12: Smaller and Smaller Length Scales for Materials Analysis

3.2.2 Short-Term Nuclear Materials Development Needs

The Nuclear Materials Breakout session discussed the needs and issues associated with materials development and testing. The materials are exposed to the same environment as fuels and, therefore, have been analyzed in a similar way. Mechanical testing of the pressure vessel metals for LWRs as well as for the next generation of nuclear power plants is an issue. The ability to measure performance at high dose is needed as well as the ability to validate models for future extension to longer life by studying microstructures.

Proper Microstructural Characterization. Property and microstructure relationships need to be evaluated and established to move beyond empirical based testing. Mechanistic understanding is required to move beyond the current empirically based NRC regulations.

Atomic Scale Effects. It is necessary to understand irradiation effects at very small scales such as radiation induced segregation, grain boundary effects, trace element analysis, and void swelling.

In-situ Measurements. The ability to evaluate deformation mechanics, damage development, annealing studies, and other time resolved measurements is needed to gain the real time evolution of these phenomena rather than being limited to discreet time steps based on irradiated samples.

Full Physical/Mechanical Properties with Environmental Control. Reliable data is needed to fill in gaps concerning fatigue, creep, and creep fatigue on irradiated materials.

Irradiation Assisted Stress Corrosion Cracking (IASCC). Reliable data is needed to evaluate the environmental conditions associated with corrosion cracking for higher activity materials (see Figure 13).

Environmental Assisted Fatigue. Reliable data is needed to evaluate environmental assisted fatigue on high activity materials.

Samples for Testing. The capability to prepare samples from highly activated materials is critical to subsequent analysis and examinations. Preparing samples out of irradiated materials for hot work and making very small samples for testing in non-irradiation areas are two issues.

Ability to Move Samples. Because irradiation testing and PIE capability are distributed, there is a need to simplify and standardize shipping containers, sample containers, and instrument sample holders to resolve inter-laboratory incompatibility and reduce complexity due to shipping regulations.

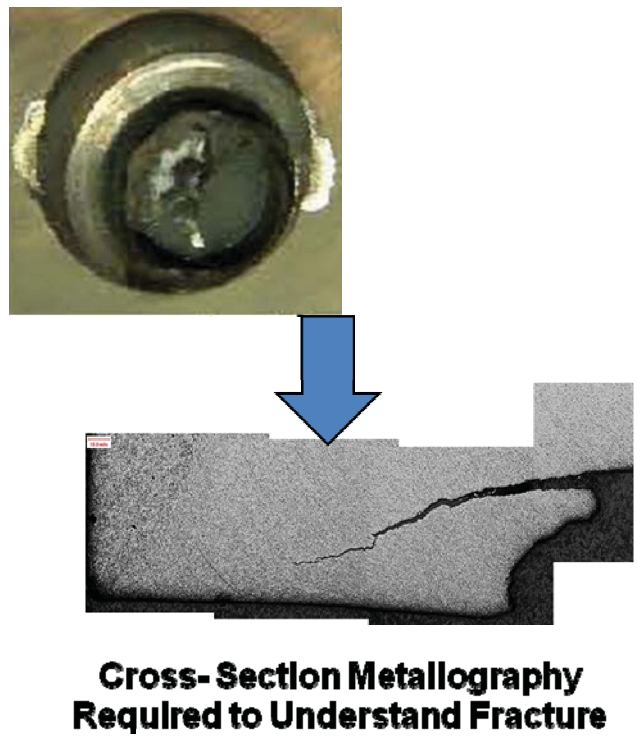


Figure 13: Reactor Internals (Stainless Steels) -- Plant Materials Assessment

3.2.3 Long-Term Nuclear Materials Development Needs

In-situ Everything. In-situ measurements are needed to evaluate dynamic microstructure changes in materials along with deformation development and surface effects development. Further in-situ measurements support in cell measurements of systems and near pile characterization of strain. This in-situ characterization shows development and time scale compared to static PIE and feeds well into modeling efforts.

High Dose > 200 DPA Materials. Characterization of high dose materials is needed to validate models to very high doses. Currently data for materials over 200 DPA does not exist. It is likely that such materials may have unique structures (e.g. composites) which may require development of special examination equipment and techniques.

3.2.4 Conclusions

The Nuclear Materials Breakout Session identified several needs supporting the development of materials and fuels. The ability to study materials at the micro-scale and in-situ are the major technology driven needs. Access to the testing facilities is needed. Transportation issues must be resolved for irradiated materials, including samples.

3.3 Modeling & Simulation/Scientific Measurements

The Breakout Session for Modeling & Simulation (M&S) / Scientific Measurements discussed PIE and characterization needs.

3.3.1 Modeling and Simulation Description

Over the past two decades, the U.S. has developed and deployed the world's most powerful collection of tools for the synthesis, processing, characterization, and M&S of materials and chemical systems at the nanoscale (dimensions of a few atoms to a few hundred atoms across). These tools, which include world-leading x-ray and neutron sources, nanoscale science facilities, and high-performance computers, provide an unprecedented view of the atomic-scale structure and dynamics of materials and the molecular-scale basis of chemical processes. For the first time in history, we are able to synthesize, characterize, and model materials and chemical behavior at the length scale where this behavior is controlled.

While the use of these advanced tools has gained traction in materials research for other industries such as photovoltaics, their use is still limited for irradiated materials characterization. Harnessing the potential of computational science and engineering for the discovery and development of materials and chemical processes is essential to maintaining leadership in these foundational fields. Simulation-based engineering and science in materials and chemistry will require an integration of experimental capabilities with theoretical and computational modeling; the development of a robust and sustainable infrastructure to support the development and deployment of advanced computational models; and the assembly of a community of scientists and engineers to implement this integration and infrastructure. [11]

"The confluence of new theories, new materials synthesis capabilities, and new computer platforms has created an unprecedented opportunity to implement a "materials-by-design" paradigm with wide-ranging benefits in technological innovation and scientific discovery." [11]

The knowledge and data gained under the experimental and theoretical elements of the science-based approach will be incorporated into an advanced M&S program that takes advantage of state-of-the-art computing capabilities. Due to the very complex nature of the licensing process for nuclear fuels, a formal science-based approach must be developed and implemented to demonstrate the validity of the newly developed simulation tools to address the behavior of fuels and materials in realistic situations and qualify these tools for the licensing process.

The technical objective of the modeling and simulation effort is to provide insight into highly non-linear, coupled, multi-physics processes that occur during fuel fabrication and fuel performance (see Figure 14). The practical objectives are to:

- Minimize the number of empirical iterations during fabrication and high-dose irradiation testing of fuels by designing the performance into the fuel at the early development phases

- Reduce the number of prototypes and large-scale experiments needed before demonstration and deployment
- Quantify uncertainties for design and operational parameters." [12]

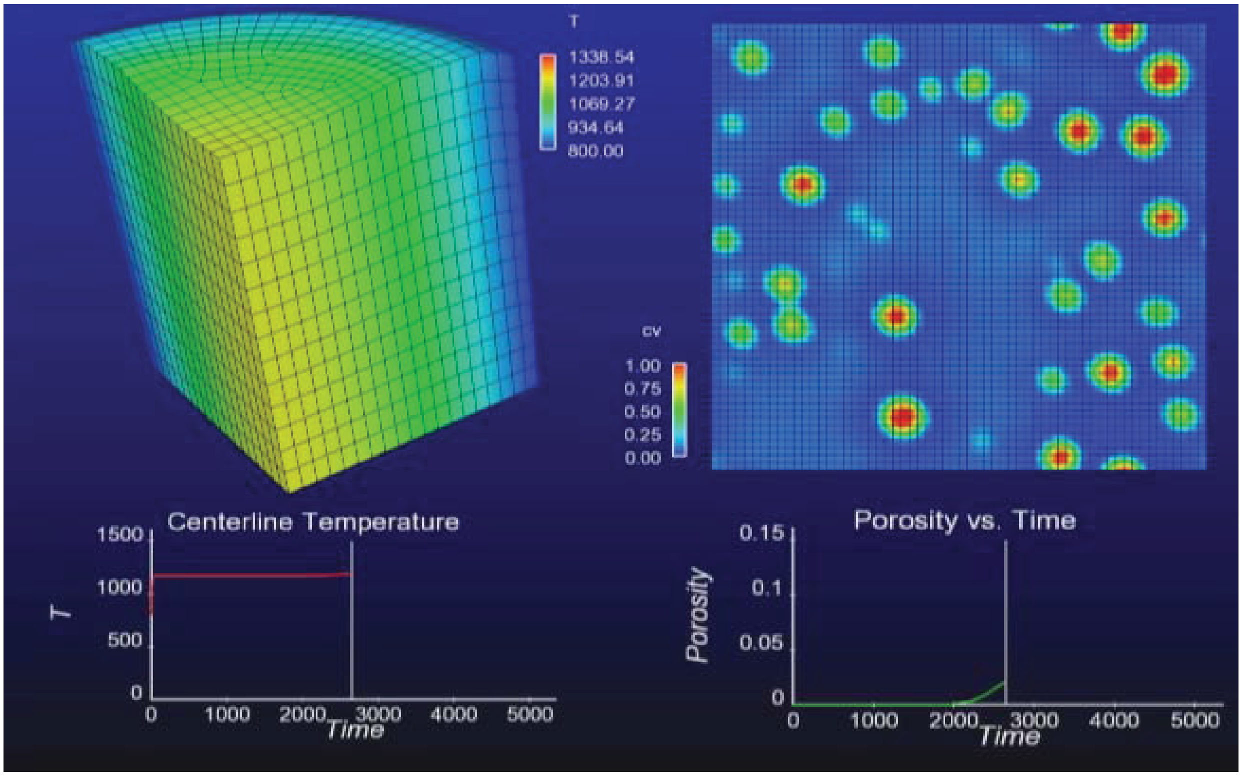


Figure 14: Evolving Microstructure Used to Degrade Thermal Conductivity - Direct Coupling of Engineering and Meso-scales

3.3.2 Scientific Measurements Description

To achieve the breakthroughs needed to understand the atomic and molecular processes that occur within the bulk and at surfaces in materials in extreme environments will require advances in the final two cross-cutting areas, characterization and computation. Identifying changes in structure and dynamics over broad timescales (femtoseconds to many seconds) and length scales (nanoscale to macroscale) is critical to developing the revolutionary materials required for future energy technologies. Advances in characterization tools, including diffraction, scattering, spectroscopy, microscopy, and imaging, can provide this critical information. The combination of two or more of these characterization tools permits so-called "multi-dimensional" analysis of materials and surfaces in-situ. [6]

Small-scale integral testing combined with scientifically developed scaling laws may alleviate the need for full-scale experiments. Novel measurement techniques with high spatial resolution (micron to sub-micron scale characterization) are needed for science-based fuel development. Finally, in-situ instrumentation for in pile experiments will be valuable to understand the transient in pile behavior of the fuels and materials." [12]

3.3.3 M&S/Scientific Measurements PIE and Characterization Needs

The M&S/Scientific Measurements Breakout Session clarified that the basis for modeling and simulation is the influence of composition and microstructure in determining properties, which in turn determines material performance. Both composition and microstructure evolve during irradiation. Thus, modeling efforts are centered on predicting microstructure evolution and the resulting properties during irradiation.

Detailed measurements are needed (i.e., at the necessary resolution) of the composition and microstructure of fuels and materials that have undergone irradiation to inform and validate models being developed to predict the evolution of microstructure under irradiation (see Figure 15). Instrument and technique development is needed to support microstructure analysis to get the resolution and detection limits.

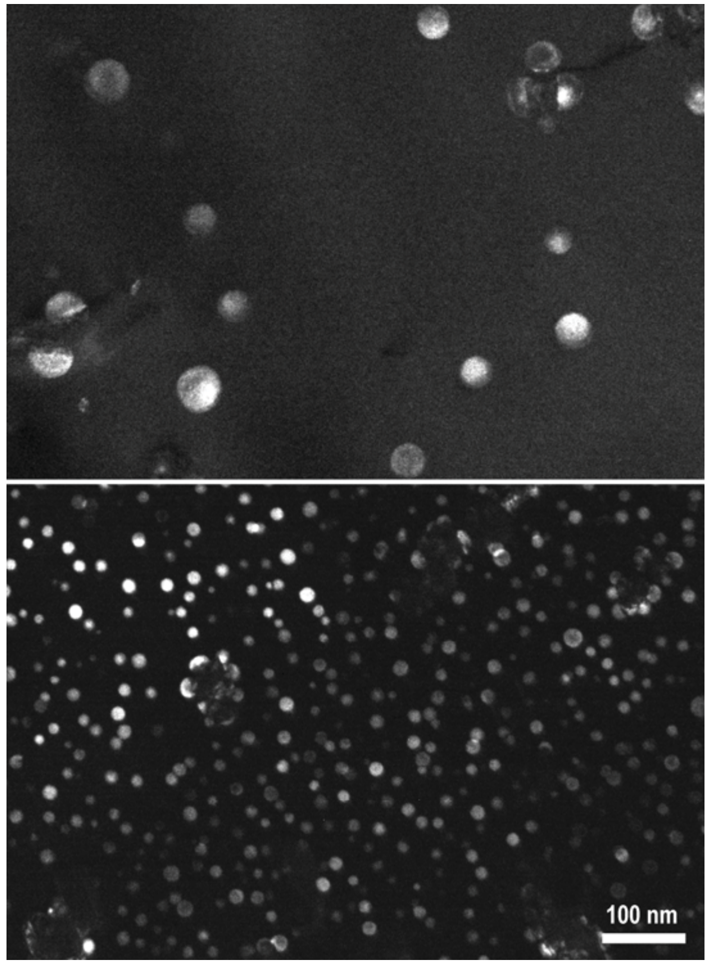


Figure 15: TEM Image, Weak beam dark field images showing comparison of irradiation-induced precipitates in the alloy 800H irradiated with neutrons in the Advanced Test Reactor at 500ºC to 1.3 dpa (top) and 800ºC to 1.5 dpa (bottom).

Two categories were evident: characterization of microstructure and properties determination. PIE on irradiated fuels and materials is critical for advanced M&S. It should be noted that many of the needs, capabilities, solutions, and instruments discussed during the course of the workshop currently exist and are in operation at various DOE laboratories. Some are even in use with irradiated materials. However, they are generally not available for use with highly irradiated materials or actinide materials (irradiated or not) due to alpha contamination.

Even though the needs that were identified focus on micro- and nano-scale characterization, there remains a strong need to continue bulk property determinations. Additional needs include maintaining accurate processing and irradiation histories on materials retained for sample and data libraries, continued research on in-situ measurements, retention of the Argonne National Laboratory (ANL) Intermediate Voltage Electron Microscope (IVEM), and the overall need to study simpler systems (e.g., pure materials, simple systems, single crystals, bi-crystals) to better complement near-term modeling efforts.

Identification/Characterization of all Phases Seen at Level of Microstructure, with Properties of Each Phase Determined. To support modeling efforts, properties need to be determined for each individual phase; these measurements could be made directly, or by separate synthesis and characterization of materials.

3D Map of Defects, Defect Structures, Chemistry at Micro-to Nano-scale; Function of Temperature, Stress, Time, etc. for Both Fuels and Cladding. Examination of these defects and chemistries is needed to understand the irradiation-induced segregation and precipitation process.

Characterize Fission Gas Distribution in Fuels. This includes bubbles (nucleation, size distribution, pressure); fission gases in the matrix, where bubbles nucleate and grow; and their stability under various irradiation conditions to inform and validate fission gas release models.

Tomography at 1 micrometer scale. Tomography at very small scales is needed to understand damage evolution and failure in fuels and materials.

Characterize Thermal Conductivity/Diffusivity of Irradiated Fuels at ~1 micrometer scale. Thermal properties characterization is needed at very small length scales at resolution as fine as the finest phase present. This allows measurement as a function of temperature and correlation with phase identification and composition, etc. Thermal properties are fundamental to calculating fuel temperature, which affects many irradiation performance parameters.

Characterize Diffusivities (Bulk Diffusion, Surface Diffusion) of Important Fuel Constituents and Fission Products (Especially Fission Gases) for Important Phases/Microstructural Features as a Function of Irradiation Conditions, Composition, etc. Characterizing diffusivities is needed for validating species transport/fission gas release models.

Characterize Mechanical, Physical Properties Measured on Same Microstructure (From 3D Characterization). The ability is needed to correlate properties to the microstructure rather than properties being correlated as a function of burnup.

The short term needs identified in this area are broad and comprehensive and basically serve as the long term needs as well; more specifically, in the long term it is expected that the identified needs will be extended to more complicated material systems at ever increasing spatial resolution.

3.3.4 Conclusions

The M&S/Scientific Measurements Breakout Session concluded that their most important needs were detailed characterization of microstructure and properties data obtained at smaller length and time scales than is currently available for highly activated fuels and cladding materials. This data is critical to informing and validating ongoing modeling efforts. Despite the need for micro- and nanoscale data, retention of bulk characterization remains important. Synthesis of the nano-to bulk-scale characterization would support the development of models that relate changes in microstructure to material performance rather than relying on a correlation *based* on burnup.

4. CAPABILITY GAPS

The main capability gaps identified during the breakout sessions were the need for micro-analysis, modeling, infrastructure, and in-situ measurements. Some gaps have solutions that were proposed by the breakout sessions.

4.1 Micro-analysis

There is an increasing need to evaluate and understand microstructural characteristics and the mechanisms that cause changes to material performance as a result of changes to the microstructure. This includes smaller length and time scales on fuels and cladding materials, as the phenomena affecting material behavior under irradiation occur at nano-scale. The equipment to analyze material at this scale currently exists. However, the use of such equipment for highly radioactive materials is not easy. It requires design changes to protect the sensitive electronic components against radiation damage and also the ability to use the equipment remotely inside shielded cells. The gap is the ability to study irradiated materials in a shielded environment with very sensitive equipment that is radiation tolerant. The shielded environment will need to control the thermal, vibration, and electromagnetic interference (EMI) and radiation background. A shielded hot cell facility that meets all the requirements for using the highly sensitive equipment to conduct PIE on irradiated fuels and materials does not currently exist. Figure 16 shows a sample data from an electron atom probe that is routinely used in material science but its application to irradiated fuels and materials is limited.

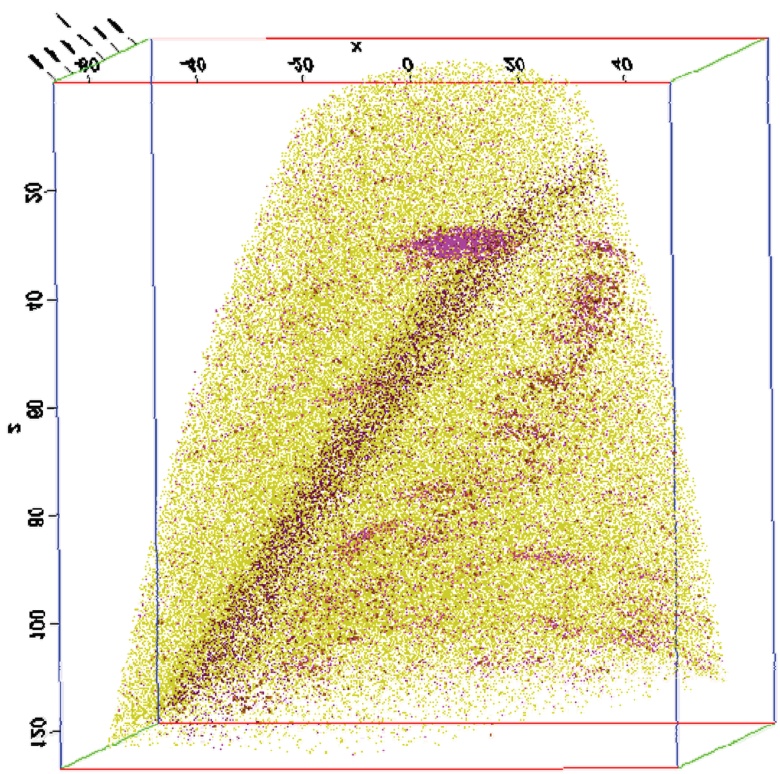


Figure 16: Local Electron Atom Probe Maps Material Composition atom-by-atom in 3D

4.2 Modeling and Simulation

Modeling and simulation tools and techniques is an essential part of science based fuels and materials development and will provide predictive behaviors of materials and allowing scientists to virtually study fuels under irradiated conditions. Validated, predictive models would significantly reduce the development time for new fuels and materials. To be predictive, the M&S tools must be able to bridge multiple decades of time- and length-scales as illustrated in Figure 17. To support the theory development and to validate the models, an advanced PIE capability is essential. However, under the science-based development paradigm, the demand on the PIE technology increases considerably:

- The ability does not exist to collect data at the micro-scale in order to better inform and validate current modeling efforts.
- The modeling community needs statistically significant data that require analyses of multiple well controlled samples.
- Traditional PIE is typically aimed at measuring dependent parameters at different length scales for comparison with model predictions. However, in order to develop and validate the models, measurements of independent parameters and separate effect phenomenology is required. For such measurements, innovative measurement techniques, which currently do not exist, must be developed.

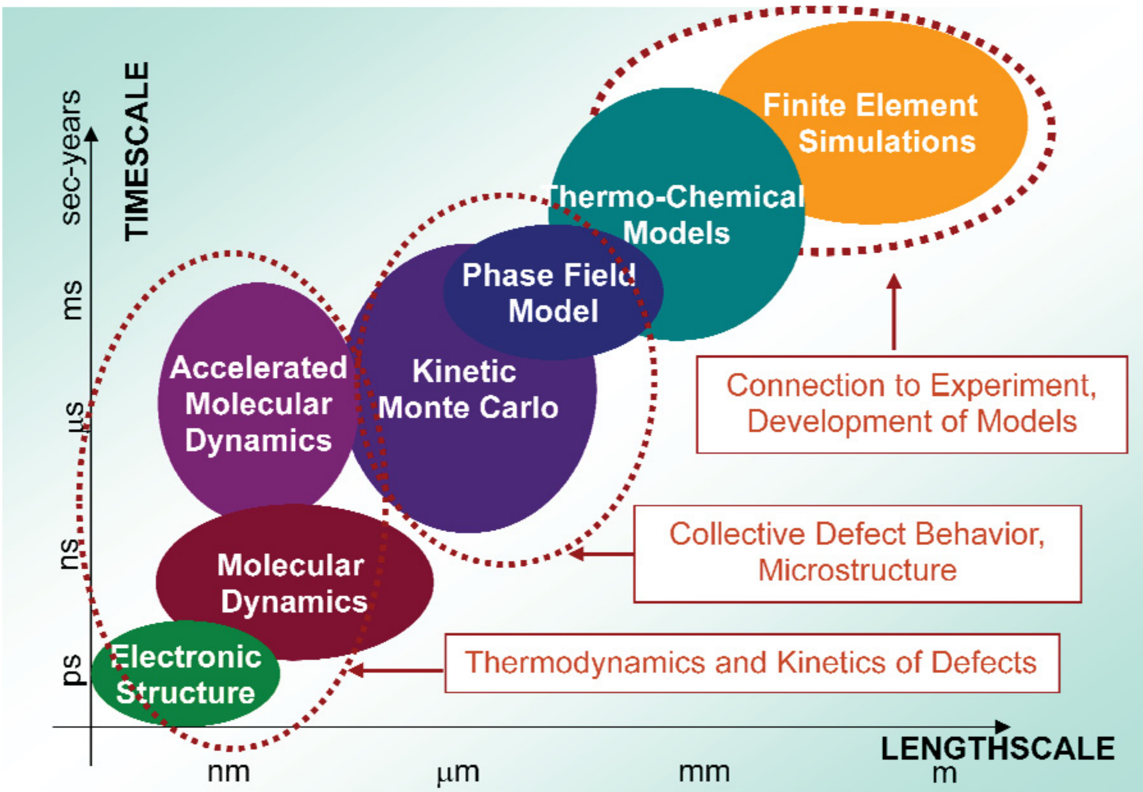


Figure 17: Multi-scale modeling of fuels and materials performance

4.3 Infrastructure

The current gap in infrastructure is the ability to examine and collect data on highly irradiated fuels and materials in a comprehensive fashion. A facility that can accommodate this type of testing with the necessary throughput does not currently exist in the United States. Much of the PIE equipment and instruments is in use for unirradiated and low activity fuels and materials. In addition, DOE national laboratories have some of the needed equipment to examine fuels at the micro- or nano-scale. However, this equipment is not capable of withstanding examinations of highly radioactive materials. A facility is needed to provide the hot-cells and shielding to examine highly irradiated fuels and materials. The shielded environment will also need the capability to control the thermal, vibration, and EMI environments. But the infrastructure gap is not just limited to examination facilities. A logical assessment of transfer between facilities and a transport infrastructure is important. In addition, the infrastructure needs to allow for sample archival, remote access to data and subsequent analyses, and a very specialized workforce to operate the highly sophisticated instruments and assess the resulting data.

4.4 In-Situ Measurements

In-situ instrumentation provides the ability to view and examine the effects of irradiation on fuel or materials while it is the reactor. If it were possible to measure all of the conditions that cause the fuel and material to degrade while under irradiation, the effects of irradiation on that material would be better understood. Another reason why in situ measurements are important is to provide the irradiation history along with all the important boundary conditions during the irradiation. Without such data, PIE only provides a snap shot in time and the results are only as good as the assumed boundary conditions and irradiation history. As such, advanced in situ instrumentation development is a very strong complement to the development of the advanced PIE capabilities.

The ability to instrument the reactor and irradiation experiments such that this type of data could be collected is only in the conceptual phase of development (except for some traditional techniques such as temperature, pressure, and flux measurements). The measurement device integrated into the reactor to measure the irradiation performance of the fuel will also be exposed to the same level of irradiation and will also undergo degradation. This effect would cause the results of the associated measurements to be suspect without calibration. In-situ measurements and analysis was a topic identified by several of the breakout sessions as the ultimate goal, acknowledging the technology development required before in-situ measurements can become a reality.

5. SUMMARY AND CONCLUSIONS

Building upon its legacy responsibilities, infrastructure, and expertise, DOE's nuclear energy mission is to perform science-based research and development focused on advanced nuclear technologies that address objectives of the NE Roadmap and promote revitalization of the nation's nuclear power industry. Over the last five years, DOE has significantly upgraded research capabilities at the INL beginning with the Advanced Test Reactor and continuing today with PIE capabilities, including a major emphasis on the installation of state-of-the-art PIE equipment and the construction of the IMCL. While some basic capabilities exist today in the U.S., DOE proposes to further invest in advanced tools and instruments for PIE that will lead to a more fundamental understanding of fuels and materials behavior.

An advanced PIE capability is crucial for the United States to maintain and further a global leadership role in advancing safe and secure nuclear energy technology. During the last 15 years, as much as the nation's nuclear research capability has been lost, nano-scale (10^{-9} meter) characterization of materials has become routine, with capabilities for sub-angstrom (10^{-10} meter) investigation becoming increasingly available to researchers in other fields. Understanding of nuclear fuel and material performance in the nuclear environment at this scale is critical to the development of the innovative fuels and materials required for tomorrow's nuclear energy systems. Existing PIE capabilities at U.S. Department of Energy (DOE) laboratories, universities, and in the private sector are widely distributed and lack the state-of-the-art capability necessary to meet the U.S. nuclear energy mission need. The DOE Nuclear Energy (NE) mission will be difficult to achieve without the availability of state-of-the-art macro-, micro-, and nano-scale characterization technology installed in a suitable radiological or nuclear facility environment. This capability will effectively harness U.S. intellectual capital by being made available to the nuclear research community as a user facility.

In addition to supporting the specific missions of DOE-NE, the capabilities resident in these advanced tools and instruments would also support forensics, nuclear attribution, and fuel development work of NNSA and National and Homeland Security, nuclear vendors, EPRI, domestic and foreign regulators, and nuclear generating companies. These capabilities will help to revitalize U.S. leadership in nuclear energy research and development and the underlying domestic nuclear science and technology infrastructure. With continuing investments to revitalize the existing infrastructure and fill mission-related capability gaps, DOE will continue to provide a national nuclear energy capability for many years to come. This capability will provide industry, universities, national laboratories, and other federal agencies with the tools required to ensure sustainable use of nuclear energy as a critical base-load power source.

With time, the number, accuracy, and spatial and temporal resolution of the parameters measured will increase as illustrated in Figure 18. To achieve the desired end state in PIE capabilities, a four-step process is envisioned.

***Step 1 – Baseline capabilities**:* The objective is to refurbish the baseline PIE capabilities within 1 to 2 years to perform PIE services for projects and programs with near-term needs. These near-term needs, developed through multiple interactions with industry, include minor equipment upgrades and catching up with necessary maintenance on existing equipment. While no new facilities are envisioned in this first step, minor upgrades will be made to existing facilities to support current capabilities. Existing equipment will be used and maintained to the extent possible to minimize schedule impacts caused by unexpected failures. During this phase, existing equipment will be analyzed to determine if it has value for future programs.

Step 2 – State-of-the Art Capabilities: The objective is to acquire new equipment and upgrade existing equipment to achieve state-of-the art PIE capabilities. With dedicated effort and stable funding, we can achieve this stage within 3 to 4 years. Some additional facility space will likely be needed to accommodate the new equipment and to streamline operations. At this point, a comprehensive set of capabilities will be available to meet the National near-term needs. However, additional capabilities would be needed to achieve world-class stature compared to international facilities that have received sustained funding and support during the previous decades (e.g. ITU in European Union). Trained staff will be recruited or developed to assure quality results and analysis.

Step 3 – World-Class Capabilities: To achieve world-class capabilities, the analysis processes and personnel expertise must be developed to a point where innovative use of equipment allows measurements possible only at a few locations in the world. The objective is to achieve this stage within 5 to 7 years.

Step 4 – World-Leading Capabilities: The objective is to develop capabilities that do not exist elsewhere for comprehensive irradiated fuels analysis. It includes recognition as leading experts, unique equipment developed in-house, and unique analyses of the data. Such capabilities will be aimed at making measurements with very small resolution (micron and sub-micron scale) at the grain and sub-grain level to support the science-based understanding of fuel behavior. At this point a complete set of facilities with adequate operational flexibility and steam-lined workflow processes will be implemented. To achieve this objective, the instrument/equipment concepts and development activities must be initiated in the near-term. Obviously, maintaining a world- leading role would require a continuous dedicated effort to stay ahead of the curve with continuous improvements beyond this point

As advanced PIE capabilities are developed, a PIE user facility will be created to build partnerships among national laboratories, universities, and industry. Most of the work can be consolidated in specific locations to minimize material transfers in large quantities and facilitate safety and security activities that are inherent with this type of work. In addition, the user facility concept would include measurements on small samples at remote locations to make best use of the overall DOE infrastructure and investments without duplicating expensive capabilities. The important features of the PIE User Facility would include the following:

- Access by national laboratories, universities, industry
- Central main facilities with distributed capabilities for specialized measurements
  - Network of facilities and capabilities
  - Data and sample archival capabilities
  - Remote access to data
  - Strategic analysis for specific locations.

This workshop was the beginning step to identify the needs towards establishing a National User Facility for characterization and PIE.

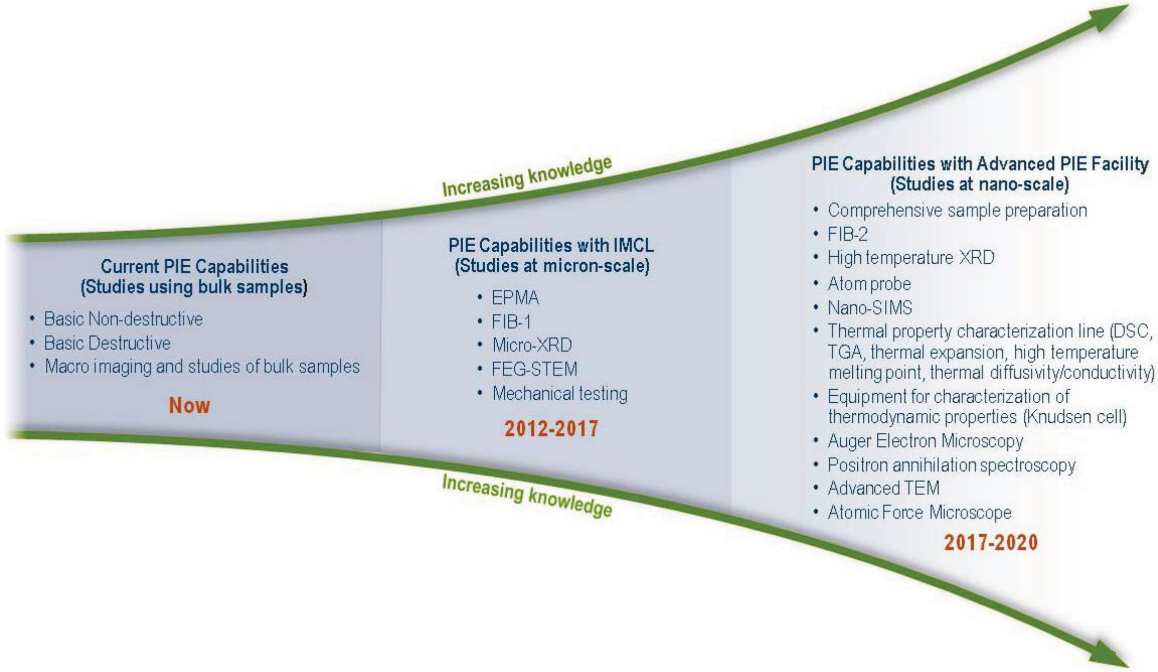


Figure 18: Transition to Advanced PIE Capability

Breakout teams identified several cross-cutting issues and four primary needs to enable accelerated innovation in PIE work and achieve DOE objectives for reactor lifespan, affordability, fuel sustainability, and proliferation. There was significant overlap in the needs and issues identified by the different participating organizations. The driver for advanced PIE and characterization capability is the need to develop and qualify nuclear fuels and materials in shorter time frames. The four primary needs are listed below:

1. Instrumentation that supports characterization of irradiated fuels and materials at the nanoscale to support increasing knowledge of mechanisms that cause material degradation. As such, an advanced PIE facility that incorporates strict environmental controls (vibration, electro-magnetic interference, temperature, etc.), environmental testing of materials (e.g., high temperature testing), sample storage and preparation adjacent to irradiation facilities, and PIE capabilities to support the advanced characterization tools is critical.

2. Advanced characterization capabilities, coupled with state of the art modeling and simulation, are needed to develop better and more predictive models, thus reducing the need for extensive empirical integral effects testing.

3. Accessibility to infrastructure and administrative systems to facilitate collaborations with participating organizations. This includes the physical infrastructure to perform PIE on highly activated fuels and materials along with administrative systems that are flexible to deal with entities (national laboratories, industry, universities) and projects (experiments, deadlines, reactor timelines, personnel career scales) that have different time cycles. This would support the development, hiring, and retention of nuclear material R&D talent.

4. Development of in-situ measurement techniques, analysis, and instrumentation that supports real-time data acquisition for deformation mechanics, damage development, and other time resolved measurements. In-situ measurements offer the potential to reveal the evolution of material attributes with time, in contrast to traditional PIE techniques that result in a small number of data points at discreet time intervals.

DOE currently has some of the resources to perform nanoscale characterization and modeling; however, the technology gaps identified during the workshop cannot be filled within the current constraints of existing laboratories. The workshop results support a user facility concept with advanced characterization and PIE capabilities to meet many of the identified needs. Advancements in modeling will come as better data obtained through advanced characterization is used to inform and validate models. Closing the gaps for infrastructure and accessibility will occur as a user facility is developed and participants benefit from collaborations. Finally, closing the gap for in-situ analysis through the development of in-pile instrumentation and dedicated beam lines will provide much greater understanding of the dynamic changes that occur in fuels and materials. The following DOE statement highlights the benefit of these advancing technologies:

> *"The confluence of new theories, new materials synthesis capabilities, and new computer platforms [which more recently has been dubbed the goal oriented, science based approach] has created an unprecedented opportunity to implement a 'materials-by-design' paradigm with wide-ranging benefits in technological innovation and scientific discovery."* [11]

The breakout sessions assembled in the national PIE workshop identified the characterization and PIE needs for nuclear energy research as well as the gaps to achieving the fundamental capabilities that would likely have high impact on enabling nuclear energy systems. Many of the identified needs can be filled using existing, commercially available technologies, provided they are adapted to work in highly radioactive environments. Advanced PIE and characterization capabilities play a significant role in achieving National nuclear energy goals and would have a dramatic impact on securing nuclear energy as a sustainable component of the national energy portfolio.

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Appendix A
Meeting Output – Fuel Development

The three fuel development breakout sessions generated similar information; therefore, they have been combined into one appendix. The three sessions are as follows:

- FCRD/Fast Reactor Fuels
- Light Water Reactor Fuels
- Gas Cooled Reactor/Particle Fuels

FCRD/Fast Reactor Fuels

Technical needs were identified and then binned into the following categories: chemistry, microstructure, properties, and integral measurements. For each category, additional discussions included spatial resolutions (maintain current integral engineering-scale measurements and increase capability in smaller length scale measurements); increased throughput, reliability, and quality (statistical and separate effects testing), and sample storage (separate effects tests and archival samples); increased modeling combined with the additional capabilities in measurement; and the ability to target regions for detailed analysis.

The specific needs for each category are identified as follows

Chemistry (Fuel and Cladding)

- Isotopics (content and distribution, submicron spatial, some temporal resolution)
- Composition (actinides, stoichiometry, fission products [FP], fission gases [FG])
- Phase (content and distribution)
- Boundaries/interfaces (system level and microstructure level)

Microstructure (Fuel and Cladding)

- Grain size and distribution (orientation, morphology)
- Void/pore/bubble distribution (morphology)
- Phase content and distribution (fuel phases, solid FP ppts)
- Defects (inclusions, surfaces, line, point: 3D→0D)
- Generally ~10 nm

Properties (Fuel and Cladding)

- Thermochemical
  - Melt point (±10°C)
  - Thermal conductivity
  - Thermal expansion
  - Specific heat
  - Vapor pressure
- Thermomechanical

  - Strength
  - Ductile-Brittle Transition Temperature (DBTT)
  - Hardness
  - Creep
  - Swelling
  - Stress/strain distribution
- Controlled atmosphere for all (e.g., dynamic operations and maintenance [O/M] control)
  - Tmax ~ 2800°C

Integral Measurements (Fuel and Cladding)

- Gross scale
  - Assembly performance (length, bow, dilation)
  - Chemistry
  - Microstructure
  - Properties
  - Reconstitution capability.

The FCRD/Fast Reactor Fuels Breakout Team also identified logistical needs for sampling and hot cells:

Logistics: Sampling

- Throughput (time to sample, ease of maintenance)
- Low cost per sample
- Uniform, automated sample preparation
- Large and small sample transport
- Disposal and waste management
- Ease of removal from experiment container
- Variety of fuel and bond materials (metallic plus sodium, graphite fuels)

Logistics: Hot Cells

- Flexibility to reconfigure for different activities
- Ability to isolate areas in cell
- Enhanced visualization for operations (e.g., Wii)
- Next generation remote operations
- In-cell cooling
- Cell/isolated area environmental control (atmosphere, temperature, purity, moisture)
- Cask handling (small to large)
- Ability to handle/measure/disassemble full assemblies

- Reconstitution capability (pins/experiments)
- Fuel & bond handling capability (sodium/lead, etc.).

Additional needs that were identified but not discretely categorized included the following:

- Long-term
  - NDA (all measurements)
  - In-situ measurements (specialty designed test situations)
- Sample uniformity
- Axial and radial measurements
- Advanced NDE to target in-depth analysis (locate the place to cut)
- Advanced NDE is critical for future transient testing
- Identification of the elements in irradiated fuel at microscale (all fission products, sodium cladding constituents, chemical states). This overlaps with fission gas and can be developed in the short term, but to get to the greater scales will be long term. The ability to analyze irradiated materials is needed (hot instruments).
- Advanced NDE Tomography
  - Visual picture of gross flaws (near-term)
  - Harvest density changes, chemicals (elemental, isotopic), dimensions, and microstructure
  - Cave rendering (long-term)
  - Image a full assembly
  - Measure initial state; condition before transient test; condition after transient
  - NDE imaging/higher resolution – measure clearly distinct fuel from cladding/structural material over the length of the disruptive zone.

The following general needs were identified for infrastructure: increased throughput of samples, remote access and communication, advancements in hot cell capabilities, transportation, and disposal/waste management. Additional details include:

- In-cell cooling capability to increase throughput; samples from irradiation to hotcell without cooling
- Capability to archive samples in a controlled environment
- Cask Handling – small to large and all types
- Remote transmittal of data
- Remote communication with operator
- Non-manipulator controlled remote operations (e.g., joystick, electronic development)
- Experiment handling
  - "Clean" or easy removal of sample from container
  - Ability to "see" the sample (new technology)

- Combine modeling with visual
  - Translate human movement to machine
  - Ease training requirements
  - Allow individuals with minimal training to use cell
- Hot cell flexibility to accommodate various activities
- Hot cell space for various activities
  - Isolate areas in-cell (temporary; keep cells clean)
  - Different cells and sizes
- Throughput, reliability, resolution
  - Quantity
  - Support modeling
  - Time to sample
  - Ease of maintenance
- Low cost per sample
- Sample preparation should be uniform, automated, and easy
- Transport large and small samples, fuels, materials, etc.
- Disposal/waste management.

Light Water Reactor Fuels

The LWR Breakout Team discussed and identified the challenges, opportunities, and research needs for LWR fuel development. General needs for this area included increased throughput to support significant statistical analysis of samples and the need to manage samples in a library with the proper quality assurance pedigree to support future access and reanalysis. Also identified was the need to provide better access to PIE data and a consideration that using traditional NDE methods but moving them to the field would provide a benefit to the amount of material needing to be transported as it could be disassembled and sectioned at its originating location.

While many specific technical needs were identified by the LWR team, these needs were categorized into seven short-term and one long-term area. Further, these needs were prioritized by relative importance. It is noted that some categories, such as mechanical properties, were scored lower in their ranking due to possibilities for sharing the cost burden for fulfilling the needs between the various participating entities.

Finally, while the initial use and throughput of these technical needs may be low, it is expected to grow as the techniques develop and the use of the data becomes more relevant. The seven short-term needs and one long-term need are as follows:

Short Term

1. Detailed microstructural and thermal properties data
2. Mechanical properties data
3. Ability to transport, receive, section, and analyze full length fuel rods
4. Ability to receive, store, and section large components

5. Administrative structure that supports paying customers
6. Sample library and sample analysis support
7. Remote characterization

Long Term

1. The long term needs fundamentally mirror the short term needs with the assumption that equipment and capability needs continual modernization aiming towards:
    a. In-situ and active monitoring
    b. Three dimensional nondestructive tomography
    c. Remote robotics manipulation.

Additional details related to the needs, such as the basis, proposed solutions, and gaps or barriers to successful implementation are included below.

1. <u>Detailed microstructural and thermal properties data</u>

- What is needed?
    - Fission product distributions (and associated local thermal properties)
    - Composition (bulk and GB) through the fuel
    - In-situ hydride re-orientation
    - Rim structure
- Why? Predict and model:
    - Corrosion and radiation effects in fuel & cladding
    - Weld integrity
    - Thermal conductivity
- Solutions? Provide access to modern equipment, such as:
    - Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Electron Probe Micro Analyzer (EPMA), X-ray Diffraction (XRD), metallography, Raman spectroscopy
    - Basic Metallography, Optical, and 3D analysis
    - Thermal properties measurements (direct measurement to minimize propagated errors and measurement of thin films with inclusion of environment)
    - Surface science (X-ray Photoelectron Spectroscopy [XPS], Auger Electron Spectroscopy [AES])
    - Laser ablation via Inductively Coupled Plasma Mass Spectrometry (ICP-MS)
    - Particle size (burst test, noble metal addition)
    - Synchrotron and neutron scattering facilities
    - Position specific sampling based on NDE

- Gaps?
  - Analysis equipment that will accept radioactive materials, especially fuels
  - High throughput sample preparation equipment
  - Automated data gathering and to provide statistically significant microstructural distributions.

2. Mechanical properties data

- What is needed?
  - Tensile and toughness
  - Fatigue and environmentally assisted fatigue
  - Stress Corrosion Cracking (SCC) and irradiation assisted SCC
  - Weld integrity
  - Flexion and vibration of large or full-size components
- Why is it needed? Need data to predict safety of plant performance and also during transportation and storage.
- Solutions? Provide access to modern equipment, such as:
  - Mechanical testing including environmental effects
  - Nano- and micro-indenters
- Gaps? Analysis equipment that will accept radioactive materials.

3. Ability to transport, receive, section, and analyze full length fuel rods

- What is needed?
  - Dimensional changes
  - Gamma scanning
  - Burst testing with particle capture and size measurement
  - Fission gas release, fission gas analysis
  - Safety testing (Loss-of-Coolant Accident [LOCA], melting tests)
  - Eddy current
  - Removal of specific rods from an assembly
  - Proper mockup facilities
  - Radiography
- Why is it needed? To understand integral properties of fuel rod.
- Solution? Adapt hot cells to perform the listed functions.
- Gap? Limited ability to receive and analyze full length fuel rods.

4. Ability to receive, store, and section large components

- What is needed?

- Cutting
- Milling
- Polishing
- Creating specific test specimens

- Why is it needed? Important plant components or storage container components will arrive as large sections. May need to look at response of fuel in storage.
- Solution? Add mills, Electrical Discharge Machining (EDM), saws to hot cells.
- Gap? Limited current ability to machine in cell.

5. Administrative structure that supports paying customers

- What is needed?
  - Rapid response capability to respond to urgent operational questions (failure analysis)
  - On time, on-budget project delivery
  - “Turn-key” structure with all casks, transport, data control, and payment issues well established
- Why is it needed? Absolute need for paying customers with ongoing operational needs.
- Solutions? Adapt contract mechanisms and retainer for priority response.
- Gap? Too often a new interaction is created with each new job.

6. Sample library and sample analysis support

- What is needed?
  - Sample storage (including unirradiated archive samples)
  - Quality assurance processes
  - Data storage & management
  - Continuity of intellectual property issues
  - Decon
  - Waste disposal (optimized by type)
- Why is it needed?
  - Key sample materials would be available for re-analysis as measurement techniques improve
  - Minimize disposal costs
- Solutions?
  - Develop sample libraries (physical storage, actual samples)
  - Increase records retention standards
- Gap? Robust sample library and sample handling protocols.

7. Remote characterization

- What is needed?
  - Remote isotope assay and temperature distributions
  - Locate rod breaches remotely without pulling rods from assemblies
  - Detect and locate nanoparticles from noble chemical additions or from burst testing
  - NDE of welds for technique improvement and as a precursor for finding flaws for further sectioning/isolation/examination
- Why is it needed? Save costs and exposure
- Solution? Develop this remote sensing capability
- Gap? Existence of this remote sensing capability

The long-term needs fundamentally mirror the short-term needs with the assumption that equipment and capability needs continual modernization aiming towards:

- In-situ monitoring of fuel properties (creep, bowing, oxidation)
- Three dimensional nondestructive microstructural tomography to ever increasing scale
- Active monitoring of fission product transport and crack size and location distributions
- More robotics and remote nano-manipulation of samples
- Improved decision process for selection of large scale facilities for decommissioning as a function of capability, need, and cost Protection of proprietary data. Establishing methods for ensuring continuity of prioritization
- Re-examine waste disposal regulations.

Gas Cooled Reactor/ Particle Fuels

The GCR/PF breakout team discussed the difference between the needs that a project has as well as the future PIE capabilities needed of this fuel type. Discussions were limited to TRISO fuels that have been highly irradiated and the application to the Next Generation Nuclear Plant (NGNP) and the LWR fuel development. The highest need for each development area was slightly different. The Advanced High Temperature Reactor (AHTR)/Fluoride Salt-cooled High Temperature Reactor (FHR) application is long-term development. The NGNP application is focused on qualifying fuels for a helium-cooled environment, while the LWR application is a water-cooled environment and has more development that needs to be done. The AHTR/FHR application is a salt fluoride environment and has the most development needed. The eight short-term and two long term needs are as follows:

Short Term

1. Diffusion and Reactivity of FPs with SiC
2. Microstructural and Chemical Evolution of TRISO Constituents (kernel, pyrocarbons, SiC)
3. High Temperature Fuel Performance in Air/Steam.
4. Strength Testing of Intact TRISO Fuel

5. Determine Internal TRISO Gas Pressure and Gas Species
6. Measurement of High Temperature Iodine Release
7. Fission Product Distribution in Graphite
8. Environmental Testing with Non-Graphite Matrix

Long Term

1. Need for Test Assembly Corrosion (salt, water, etc.) Loop for Irradiated Fuel Form
2. Real-time evolution of TRISO Compact fuel in 3D to high burn-up.

Additional details related to the needs, such as the basis, proposed solutions, and gaps or barriers to successful implementation are included below.

1. <u>Diffusion and Reactivity of FPs with SiC</u>

   - Basis for the need: As an example, Ag release is a long-standing unresolved issue, and Pd attack is a serious threat to TRISO breach.
   - Potential Solution: Advanced micro analytical techniques (x-cut)
     - 3d high spatial resolution important
     - high resolution chemical speciation
   - Gaps/Barriers: Some of the equipment currently planned (Focused Ion Beam [FIB], etc.) will include a server. Some of the equipment currently in the complex for non-radioactive applications could accomplish the mission if certified for radioactive. Some development (e.g., 3D non-invasive) would need development.

2. <u>Microstructural and Chemical Evolution of TRISO Constituents (kernel, pyrocarbons, SiC)</u>

   - Basis for the Need: Thermochemical evolution of kernel is poorly understood and experimental definition is needed to baseline modeling. Properties of pyrocarbons are unknown, and SiC shells are the basis for TRISO fission product retention and need to be understood.
   - Solutions: Advanced microstructural and microchemical techniques, especially at lower length scale (x-cut)
     - Tomography (potentially of unique to TRISO fuel)
     - Atom Probe, Nano-Sims
   - Gaps/Barriers: Pushing both chemical state and spatial resolution limits of “out of hot cell” equipment. Both a technology gap and a lack of current in-cell equipment.

3. <u>High Temperature Fuel Performance in Air/Steam.</u>

   - Basis for the Need: Fuel performance under air and water is critical to acceptance and licensing of fuels.
   - Solutions: High Temperature air-steam furnace in cell, including continual fission gas monitoring and fission product collecting
   - Gaps/Barriers: currently unavailable but within current technology

4. Strength Testing of Intact TRISO Fuel

- Basis for the Need: SiC is the ultimate pressure vessel of FP's for TRISO fuel. We do not have a good understanding of TRISO shell strength or why fuels fail. We need to provide information to benchmark modeling on irradiated, intact fuels (not bits and pieces).
- Solutions: None Current
- Gaps/Barriers: Currently we crush shells or measure sliced fuels. Ultimately we should develop an advanced test for an integrated (intact) fuel.

5. Determine Internal TRISO Gas Pressure and Gas Species

- Basis for the Need: Evolution of FP and CO within TRISO is needed as drivers for failure prediction and to benchmark modeling.
- Solutions: Gas release by mechanical or "laser," or ion milling along with mass/gamma spec.
- Gaps/Barriers: Potential limits on resolution limits.

6. Measurement of High Temperature Iodine Release

- Basis for the Need: Iodine is most important offsite contributor to dose. We need data.
- Solutions: Facility for construction of capsule to re-irradiate fuel to build-in I-131 to extract for measurement.
- Gaps/Barriers: There is currently no facility for construction of capsules with irradiated fuels

7. Fission Product Distribution in Graphite

- Basis for the Need: Understanding fission product transport and retention in graphite.
- Solutions: Combination of existing facilities to development of a 3D gamma tomography.
- Gaps/Barriers: High resolution techniques currently unavailable.

8. Environmental Testing with Non-Graphite Matrix.

- Basis for the Need: Alternative reactor platforms have non-standard matrices and require environmental and off-normal situation (e.g., LOCA) testing.
- Solutions: Steam water interaction, etc.
- Gaps/Barriers: Low-tech but non-existing in cell.

Long Term Technical needs:

Need for Test Assembly Corrosion (salt, water, etc) Loop for Irradiated Fuel Form

- Basis for the Need: Next generation of advanced TRISO-bearing reactors could utilize fluoride salt, water, helium, etc. Mass transport and corrosion will be issues at the sample, pin, and test assembly level. Tests will need to be carried out on irradiated fuel.
- Solutions: Dedicated loops. Microstructural analysis techniques (x-cut)
- Gaps/Barriers: Low-tech, but non-existing in cell.

Real-time evolution of TRISO Compact fuel in 3D to high burn-up.

- Basis for the Need: Holy Grail
- Solutions: Improved resolution tomography. Intense small volume neutron source thermal neutron source.
- Gaps/Barriers: We’re close with the tomography. No clue on the neutron source term.

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Appendix B
Meeting Output – Nuclear Materials

The Nuclear Materials Breakout Team discussed the PIE and characterization needs for nuclear materials development. The materials are exposed to the same environment as fuels, and therefore, have been analyzed in a similar way. The needs that were discussed include the ability to measure performance at high dose and the ability to validate models for future extension to longer life by studying microstructures. The eight short-term and two long-term needs were identified, as follows:

Short Term

1. Proper Microstructural Characterization
2. Atomic Scale Effects
3. In-situ measurements
4. Full Physical/Mechanical Properties with environmental control.
5. Irradiation Assisted Stress Corrosion Cracking (IASCC)
6. Environmental Assisted Fatigue
7. Samples for testing
8. Ability to move samples

Long Term

1. In situ everything
2. High dose >200dpa materials

Additional details concerning the underlying needs for each of these categories and the basis, proposed solution, and gaps or barriers to successful implementation are included in the following.

1. <u>Proper Micro-structural Characterization</u>

- Basis for the Need: Property Structure relations
  - NRC regulations are empirical based - need mechanistic understanding
  - Mechanical Testing is mostly data right now - need deformation mechanics
- Solutions: Microscopy
- Gaps/Barriers: Full complement of modern micro-structural equipment not available for high irradiated materials

2. <u>Atomic Scale Effects</u>

- Basis for the Need: Understanding irradiation effects at small scales
  - Radiation Induced Segregation
  - Grain Boundary Effects
  - Trace Element Analysis
  - Void Swelling

- Solutions: EPMA, Atomic Force Microscopy (AFM), Secondary Ion Mass Spectrometry (SIMS), Ablation, TEM
- Gaps/Barriers: Full complement of modern micro-structural equipment not available for high irradiated materials

3. <u>In-situ measurements</u>

- Basis for the Need: deformation mechanics, damage development, annealing studies and other time resolved measurements
- Solutions: Synchrotron Access (dedicated beamlines) with tomography, diffraction, atomic pair distribution function (PDF), other high energy light source techniques
- Gaps/Barriers: Difficulty in getting high irradiated samples on existing beamlines

4. <u>Full physical/mechanical properties with environmental control</u>

- Basis for the Need: Reliable data
- Solutions: Testing machines with environmental control
- Gaps/Barriers: We are good at crack growth and tension/compression, DBTT, but are missing fatigue, creep, and creep fatigue data on irradiated materials.

5. <u>IASCC</u>

- Basis for the Need: Reliable data
- Solutions: Testing machines with environmental control
- Gaps/Barriers: Not enough equipment. Higher activity equipment

6. <u>Environmental Assisted Fatigue</u>

- Basis for the Need: Reliable data
- Solutions: Testing machines with environmental control
- Gaps/Barriers: No currently available equipment that can do high activity and tension-compression fatigue.

7. <u>Samples for testing</u>

- Basis for the Need: Need samples to test
- Solutions: Hot EDM and other machining capabilities
- Gaps/Barriers: Few warm/hot EDM's exist, not enough sample throughput. There are two problems with the samples. The first is getting samples out of irradiated materials for hot work; the second is making very small samples for testing outside of irradiated areas (e.g., universities, national labs, etc).

8. <u>Ability to move samples</u>

- Basis for the Need: Irradiation does not happen at testing sites. (old irradiations, decommissioned pieces)
- Solutions: Standardization of shipping and sample containers and instruments sample holders

- Gaps/Barriers: Inter-laboratory incompatibility, shipping regulations

Long-Term Needs

1. In-situ everything

- What is the need?
  - Dynamic Microstructure Measurements
  - Deformation Development
  - Surface effects development
  - In cell measurements of systems
  - Near pile characterization of strain
- Basis for the Need: In-situ characterization shows development and time scale vs. static PIE; feeds well into modeling.
- Solutions:
  - Dedicated beamline with high irradiated sample handling at synchrotron facilities
  - Matter-Radiation Interactions in Extremes (MaRIE) in-situ characterization during irradiation
  - Hot/Cold stage, deformation stage on microscopes (TEM, surface instruments)
- Gaps/Barriers: Funding for beamline activities

2. High dose >200dpa materials

- Basis for the Need: Validating models to very high dose; currently no extant data over 200 dpa
- Solutions:
  - Fast Reactor
  - Materials Mining from Decommissioned Reactors
  - Ion Implantation
- Gaps/Barriers:
  - Irradiation Comparison studies (scale dose temperature)
    - Ion implantation vs. Fast Reactor
    - Fast Reactor vs. LWR
  - Handling high dose materials for testing.

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Appendix C
Meeting Output – Modeling and Simulation

The M&S needs were grouped into two categories: characterization of microstructure and properties determination. The barrier to reaching or fulfilling these needs is related to a common misunderstanding within the PIE community. That being, many of the needs, capabilities, solutions, and instruments discussed during the course of the workshop currently exist and are in operation at various DOE laboratories. Some are even in use with irradiated materials. However, they are generally not available for use with highly irradiated materials or actinide materials (irradiated or not) due to fear of alpha contamination. Thus, a capability dedicated to characterizing irradiated fuels is needed.

Even though the needs that were identified focus on micro- and nano-scale characterization, there remains a strong need to continue bulk property determinations. Further, general needs identified included maintaining accurate processing and irradiation histories on materials as they are retained to meet the identified need of sample and data libraries, movement forward on in-situ measurements, retention of the ANL Intermediate Voltage Electron Microscope (IVEM), and the overall need to study simpler systems (e.g., pure materials, simple systems, single crystals, bi-crystals) to better couple with near-term modeling efforts.

Characterization of Microstructure

1. Identification/characterization of all phases seen at level of microstructure, with properties of each phase determined

    - Basis for the Need: Property measurements could be made directly? Or by separate synthesis and characterization of materials.
    - Solutions: High resolution (HR)-TEM, μXRD, FIB
    - Gaps/Barriers: Measurement of properties at fine scale is difficult; ex-reactor synthesis may not be possible.

2. 3D map of defects, defect structures, chemistry at micro- to nanoscale; function of temperature, stress, time, etc. for both fuels and cladding

    - Basis for the Need: Needed to understand irradiation-induced segregation and precipitation processes
    - Solutions: Atom probe, nano-SIMS, TEM/Scanning Transmission Electron Microscope (STEM) with Electron Energy Loss Spectroscopy (EELS), Energy Dispersive Spectroscopy (EDS) with heating & strain stage, Orientation Imaging Microscopy (OIM), stereo-imaging, micro X-ray absorption spectroscopy (μXAS; perhaps at light source)
    - Gaps/Barriers: Will light sources accommodate irradiated fuels? New configurations of systems listed may be needed. New/improved detectors for these systems may be needed.

3. Characterize fission gas distribution in fuels

    - What is the need?
        - Bubbles (nucleation, size distribution, pressure)
        - Fission gases in the matrix
        - Where bubbles nucleate and grow

   - Their stability under various irradiation conditions

- Basis for the Need: Inform and validate fission gas release models
- Solutions: TEM, SIMS, nanoSIMS, x-ray tomography, single angle X-ray scattering (SAXS), single angle neutron scattering (SANS)

4. Tomography at 1 µm scale

- Basis for the Need: Understand damage evolution and failure
- Solutions: High energy x-rays (>200 KeV), gamma-ray lasers could also enable Nuclear Resonance Fluorescence (NRF) at same time giving isotopic information
- Gaps/Barriers:
   - Perhaps neutron radiography could be used if improvements in n-detection resolution can be improved
   - Need improvements in analysis software
   - Need to increase throughput
   - Weapons program may have capability

Property Determination

1. Characterize thermal conductivity/diffusivity of irradiated fuels at ~1 µm scale
   - Resolution as fine as finest phase present?
   - Measured as a function of temperature and correlated with phase identification, composition, etc.

- Basis for the Need: Fundamental to calculating fuel temperature, which effects many irradiation performance parameters
- Gaps/Barriers: Statistical Time Division Multiplexing (STDM) currently limited to metallic samples, low temperatures

2. Characterize diffusivities (bulk diffusion, surface diffusion) of important fuel constituents and fission products (especially fission gases) for important phases/microstructural features as a function of irradiation conditions, composition, etc.

- Basis for the Need: Needed for validating species transport/fission gas release models
- Gaps/Barriers: Instrument/technique development needed; even theory may be intractable. Need to reformulate need in a manageable way.

3. Characterize mechanical, physical properties measured on same microstructure (from 3D characterization)

- Basis for the Need: Correlate properties with microstructure
- Solutions: Micro/nano-indentation, need instrument/method development
- Gaps/Barriers: How do properties determined at low-length scales correlate with engineering scale?

Appendix D
Agenda

Gaithersburg Marriott Washingtonian Center
Ballroom Room C&D

Tuesday, March 29, 2011

8:00	Welcome / Introductions	Kemal Pasamehmetoglu
8:15	Opening Remarks / Mission Need	Dennis Miotla, DOE-NE
8:45	Workshop Expectations and Purpose	Kemal Pasamehmetoglu
9:30	***Break***	
	Current and Future User Needs for PIE	
10:00	• Vendor Perspective	Michael Burke, Westinghouse
10:30	• DOE-NE Research	Steve Hayes, INL
11:00	• University – Fuel research	Sean McDeavitt, TAMU
11:30	***Lunch***	
	Current and Future User Needs for PIE	
1:00	• ATR National Scientific User Facility	Todd Allen, ATR-NSUF
1:30	• NRC PIE Perspective	John Voglewede, NRC
2:00	• Storage Concepts Evaluation Results	Ruth Weiner, SNL
2:30	***Break***	
3:00	National PIE Capability Video	Kemal Pasamehmetoglu
3:30	Breakout Sessions • FCRD / Fast Reactor Fuels • Light Water Reactor Fuels • Gas Cooled Reactor Fuel / Particle Fuels • Modeling & Simulation • Nuclear Materials	
5:30	***Welcome Meeting: Ballroom Salon G***	***Kemal Pasamehmetoglu***
	"Transforming Fuel Development into a Science Based Approach"	

Gaithersburg Marriott Washingtonian Center
Ballroom Room C&D

Wednesday, March 30, 2011

8:00	Welcome / Continue Breakout Sessions	Kemal Pasamehmetoglu
10:00	Prepare Presentations	
	Breakout Team Presentations	
11:00	• FCRD / Fast Reactor Fuels	Ken McClellan
11:30	• Light Water Reactor Fuels	Todd Allen
Noon	***Lunch***	
	Breakout Team Presentations (continued)	
1:30	• Gas Cooled Reactor / Particle Fuels	Lance Snead
2:00	• Modeling & Simulation	Steve Hayes
2:30	• Nuclear Materials	Tarik Saleh
3:00	Summary Discussion / Path Forward	Kemal Pasamehmetoglu
3:30	***Adjourn***	

Appendix E
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