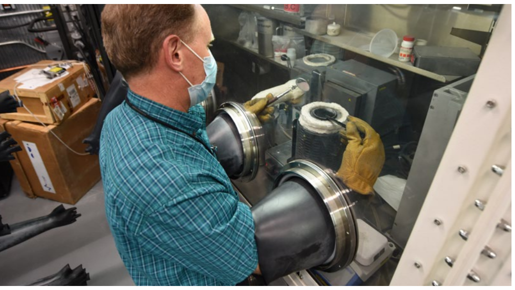
INL/EXT-21-62001

ANNUAL REPORT

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Idaho National Laboratory



LETTER FROM INL'S CHIEF RESEARCH OFFICER

The Department of Energy's (DOE) Laboratory Directed Research and Development (LDRD) program is an essential pathway for innovation and capability growth at Idaho National Laboratory (INL). LDRD enables agile responses to the national energy challenges that motivate INL's mission to discover, demonstrate, and secure innovative nuclear energy solutions, clean energy options, and critical infrastructure. INL's LDRD program sustains and enhances the technical vitality of INL's core capabilities by advancing the frontiers of science, technology, and engineering, serving as a proving ground for new concepts, exploring revolutionary solutions to emerging challenges, and reducing the risk of technology surprise. LDRD projects also attract, develop, and retain tomorrow's technical workforce in mission critical areas of expertise.

INL's LDRD portfolio has experienced steady growth in recent years, increasing from $23 million in fiscal year (FY) 2017 to $34 million in FY 20, with further growth anticipated over the next several years. We apply a rigorous review and selection process to identify innovative, high-impact research projects that support INL's mission and are focused on communicating the impact of our LDRD research.

Dr. Marianne Walck

DEPUTY LABORATORY DIRECTOR, SCIENCE AND TECHNOLOGY AND CHIEF RESEARCH OFFICER

IDAHO NATIONAL LABORATORY

This report highlights INL's LDRD projects concluding in FY 20, which included innovative research and development (R&D) across INL's five science and technology (S&T) initiatives: nuclear reactor sustainment and expanded deployment, integrated fuel cycle solutions, integrated energy systems, advanced design and manufacturing for extreme environments, and secure and resilient cyber-physical systems.

For example, research funded through LDRD supported the sustainment of the existing fleet of nuclear reactors and the future deployment of advanced reactors by developing new modeling and simulation tools and improving test bed capabilities in the Advanced Test Reactor (ATR) and the Transient Reactor Test Facility (TREAT). LDRD investment improved techniques to evaluate advanced fuels and developed innovations in long-term wet or dry storage of spent nuclear fuel to advance integrated fuel cycle solutions. A project focusing on the low-carbon energy options needed for the integrated energy systems of the future identified novel technologies for subsurface thermal storage. INL acted quickly to direct LDRD resources towards the national coronavirus disease 2019 (COVID-19) response by funding the design of an advanced prototype auxiliary device to purify respired air on any existing ventilator, leveraging INL's unique capabilities in advanced design and manufacturing for extreme environments. LDRD research done to ensure secure and resilient cyber-physical systems will have real-world implications for the security of wireless vehicle charging and nuclear safeguards.

INL's LDRD program exhibited resiliency in 2020, adapting in the face of COVID-19 related challenges. Work on projects continued, and proposal calls and reviews proceeded on schedule.

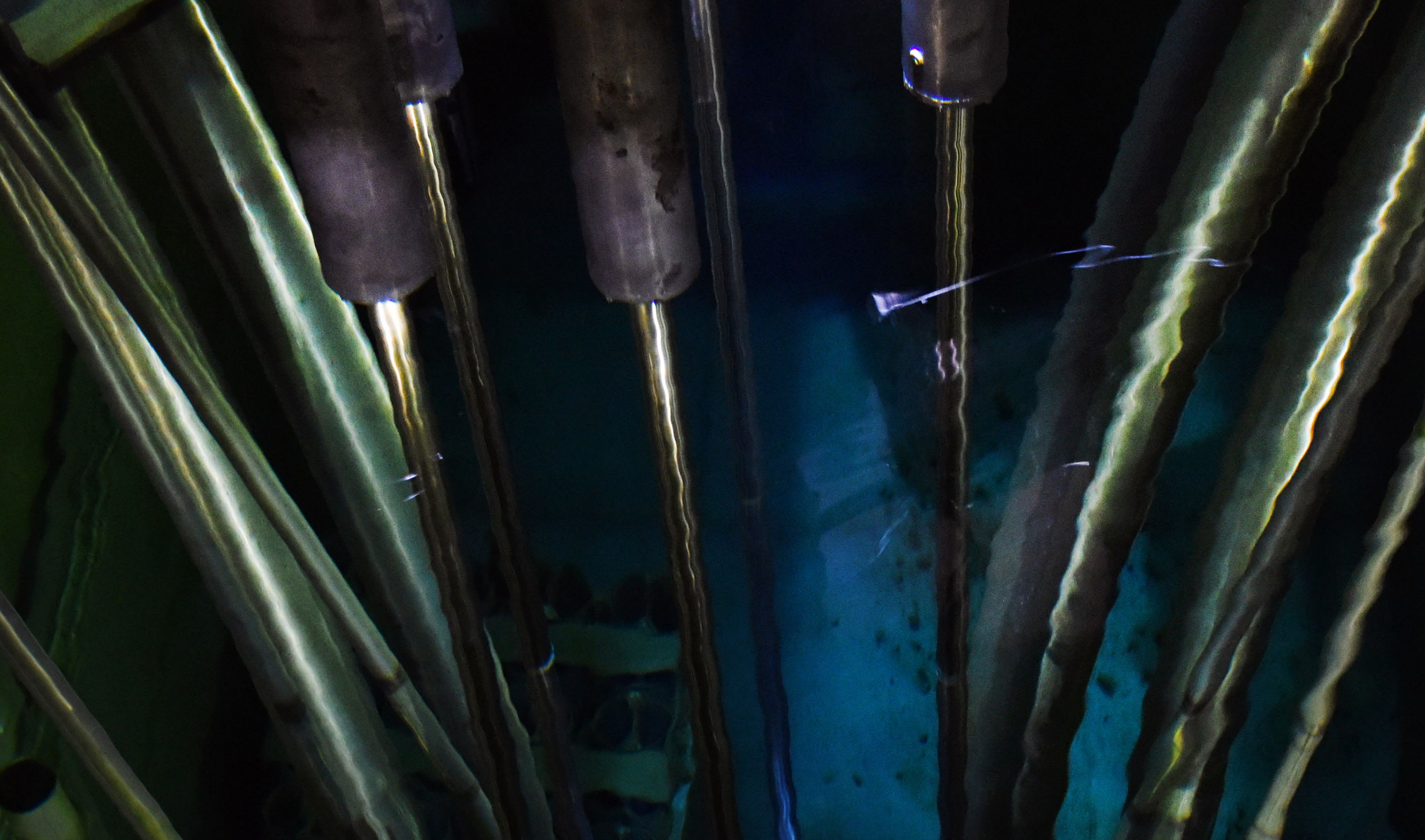
I am particularly proud that the Laboratory continued to onboard interns virtually and engage them in projects remotely. Even our annual LDRD poster session was successfully conducted virtually giving researchers the opportunity to showcase their work to stakeholders from across INL and beyond.

INL will continue to invest in LDRD to support our world-class staff and deliver the research, development, and demonstration (RD&D) our nation needs to address its energy and security challenges, now and into the future. I invite you to review this report to see how INL's LDRD portfolio enables innovation and builds the talent pipeline to advance INL's vision to change the world's energy future and secure our critical infrastructure.

TABLE OF CONTENTS

ACRONYMS & ABBREVIATIONS

2D	two-dimensional
3D	three-dimensional
4D	four-dimensional
5G	fifth generation
AM	additive manufacturing
ASR	alkali-silica reaction
ATR	Advanced Test Reactor
COVID-19	coronavirus disease 2019
DIAMOND	Data Integration Aggregated Model for Nuclear Deployment
DOE	Department of Energy
DOE-ID	Department of Energy Idaho Operations Office
DPD	Dissipative particle dynamics
ENDP	electrochemical non-oxidative deprotonation
FTM	facilitated transport membrane
FY	fiscal year
GPU	graphics processing unit
HALEU	high-assay low-enriched uranium
HEPA	high-efficiency particulate air
HPC	high-performance computing
HR-ICP-MS	high resolution inductively coupled plasma mass spectrometer
ICS	industrial control systems
IDR	invention disclosure records
INL	Idaho National Laboratory
LDRD	Laboratory Directed Research and Development
LENS	laser-engineered net shaping
LLNL	Lawrence Livermore National Laboratory
MASTODON	Multi-hazard Analysis for STOchastic time-DOmaiN phenomena
MFC	Materials & Fuels Complex
MIT	Massachusetts Institute of Technology
mmWave	millimeter wave
MOC	method of characteristics
MOOSE	Multiphysics Object-oriented Simulation Environment
MSR	molten salt reactor
NMR	nuclear magnetic resonance
NRC	Nuclear Regulatory Commission
NTP	nuclear thermal propulsion
ORNL	Oak Ridge National Laboratory
R&D	research and development
RF	radio frequency
RD&D	research, development, and demonstration
S&T	science and technology
SDR	software disclosure record
SEND	scanning electron nanodiffration
SPS	spark plasma sintering
STEM	scanning transmission electron microscope
TEM	transmission electron microscopy
TMP	thermomechanical processing
TREAT	Transient Reactor Test Facility
U.S.	United States
VESIL	Versatile Experimental Salt Irradiation Loop
Virginia Tech	Virginia Polytechnic Institute and State University
WPT	wireless power transfer

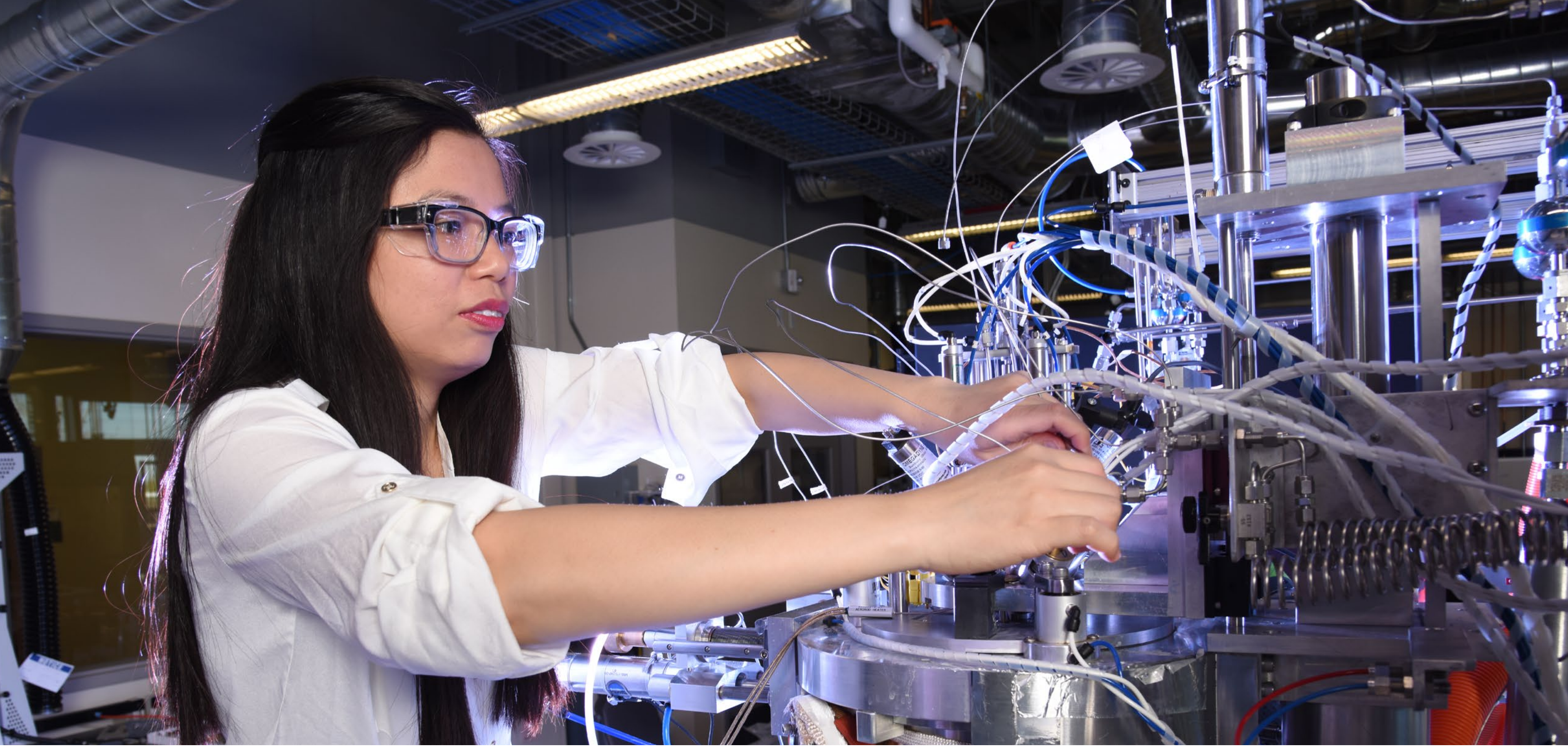


PERIODIC TABLE OF ELEMENTS

- Alkali metal
- Alkaline earth metal
- Actinide
- Lanthanide
- Transition metal
- Post-transition metal
- Metalloid
- Reactive Nonmetal
- Noble gas
- Unknown

												He Helium
							B Boron	C Carbon	N Nitrogen	O Oxygen	F Fluorine	Ne Neon
							Al Aluminium	Si Silicon	P Phosphorus	S Sulfur	Cl Chlorine	Ar Argon
Cr Chromium	Mn Manganese	Fe Iron	Co Cobalt	Ni Nickel	Cu Copper	Zn Zinc	Ga Gallium	Ge Germanium	As Arsenic	Se Selenium	Br Bromine	Kr Krypton
Mo Molybdenum	Tc Technetium	Ru Ruthenium	Rh Rhodium	Pd Palladium	Ag Silver	Cd Cadmium	In Indium	Sn Tin	Sb Antimony	Te Tellurium	I Iodine	Xe Xenon
W Tungsten	Re Rhenium	Os Osmium	Ir Iridium	Pt Platinum	Au Gold	Hg Mercury	Tl Thallium	Pb Lead	Bi Bismuth	Po Polonium	At Astatine	Rn Radon
Sg Seaborgium	Bh Bohrium	Hs Hassium	Mt Meitnerium	Ds Darmstadtium	Rg Roentgenium	Cn Copernicium	Nh Nihonium	Fl Flerovium	Mc Moscovium	Lv Livermorium	Ts Tennessine	Og Oganesson

Nd Neodymium	Pm Promethium	Sm Samarium	Eu Europium	Gd Gadolinium	Tb Terbium	Dy Dysprosium	Ho Holmium	Er Erbium	Tm Thulium	Yb Ytterbium	Lu Lutetium
U Uranium	Np Neptunium	Pu Plutonium	Am Americium	Cm Curium	Bk Berkelium	Cf Californium	Es Einsteinium	Fm Fermium	Md Mendelevium	No Nobelium	Lr Lawrencium



LDRD OVERVIEW

INL's LDRD Portfolio

LDRD is a vital DOE program that allows INL and other DOE laboratories to support a limited number of select research, development, and demonstration (RD&D) projects.[1] It works to: 1) maintain the scientific and technical vitality of INL, 2) enhance INL's ability to address future DOE missions, 3) foster creativity and stimulate exploration of forefront S&T, 4) serve as a proving ground for new research, and 5) support high-risk, potentially high-value RD&D. INL's investment in LDRD advances DOE's goals in energy, security, and the environment, with specific focus on investing in earlier-stage, higher-risk RD&D projects.

LDRD investments are used to further integrate and apply INL's strengths in basic and applied RD&D projects. These innovative projects offer the potential to advance INL's five S&T initiatives and core capabilities by focusing on both long-term objectives and key S&T drivers. Additionally, strategic investments enable researchers to conduct early-stage exploratory research to foster innovation through collaborative RD&D and provide science and engineering opportunities for students and postdoctoral researchers.

INL's LDRD portfolio comprises three investment components: the Strategic R&D fund, the Seed fund, and the Distinguished Postdoctoral Fellowship fund. The Strategic R&D fund addresses research priorities to fill S&T gaps to advance INL S&T initiatives. The Seed fund allows researchers to advance innovative ideas that require some measure of refinement before becoming fully developed, to demonstrate initial proof of concept, or to acquire data to support an application for future funding. The Distinguished Postdoctoral Fellowship fund supports work by early career researchers in INL's three distinguished postdoctoral fellowships and grows INL's talent pipeline by attracting and retaining promising early career researchers.

LDRD investments are continually aligned with INL's vision, mission, and S&T initiatives. The diverse LDRD portfolio explores a range of scientific and engineering concepts through technically sound, innovative, and cutting-edge RD&D projects. INL's LDRD research stimulates exploration at the forefront of advanced reactor modeling, nuclear waste reduction, fuel recycling, cybersecurity, electric grid reliability, and wireless technology. The Lab's innovative RD&D supports the DOE mission by advancing integrated energy systems and evolving energy security needs.

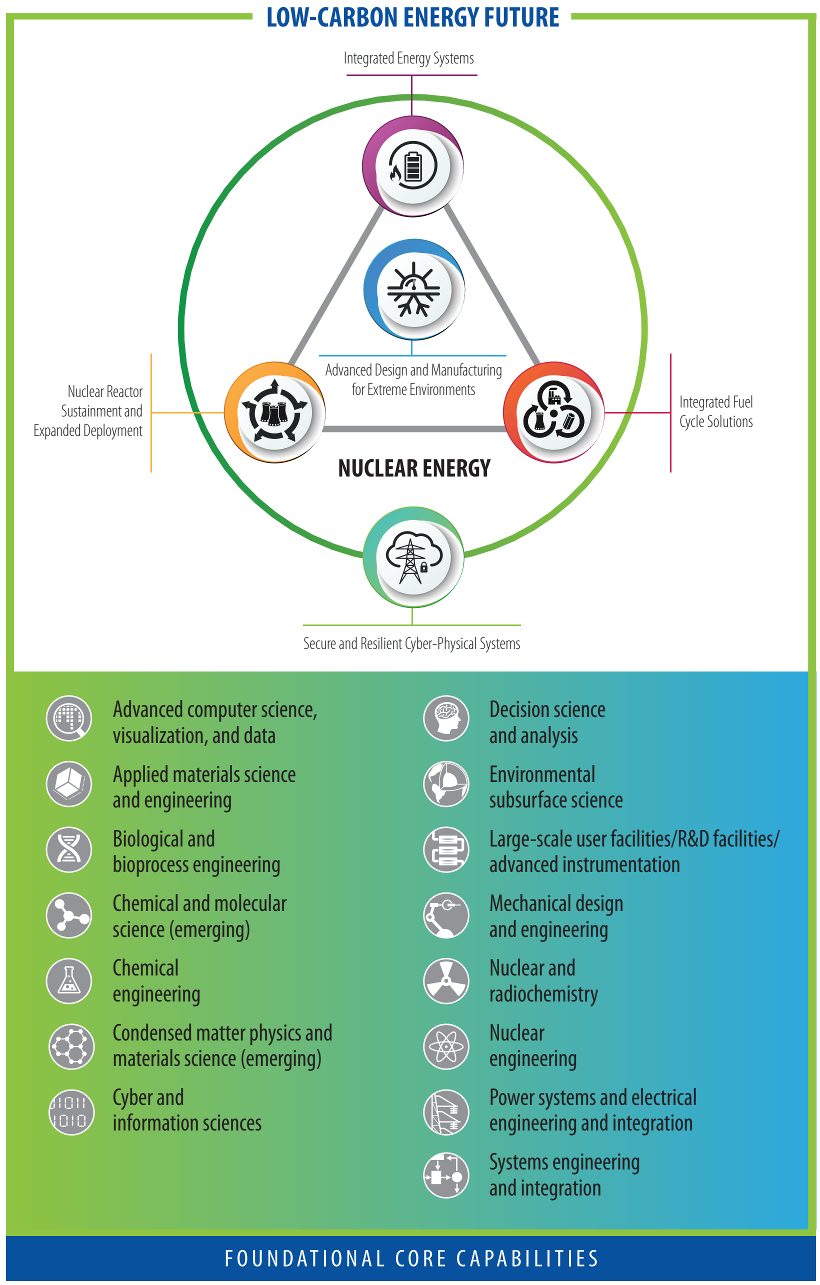
1 Please note that, due to space constraints, only select project products are included in this report. Papers in the review process are not included.

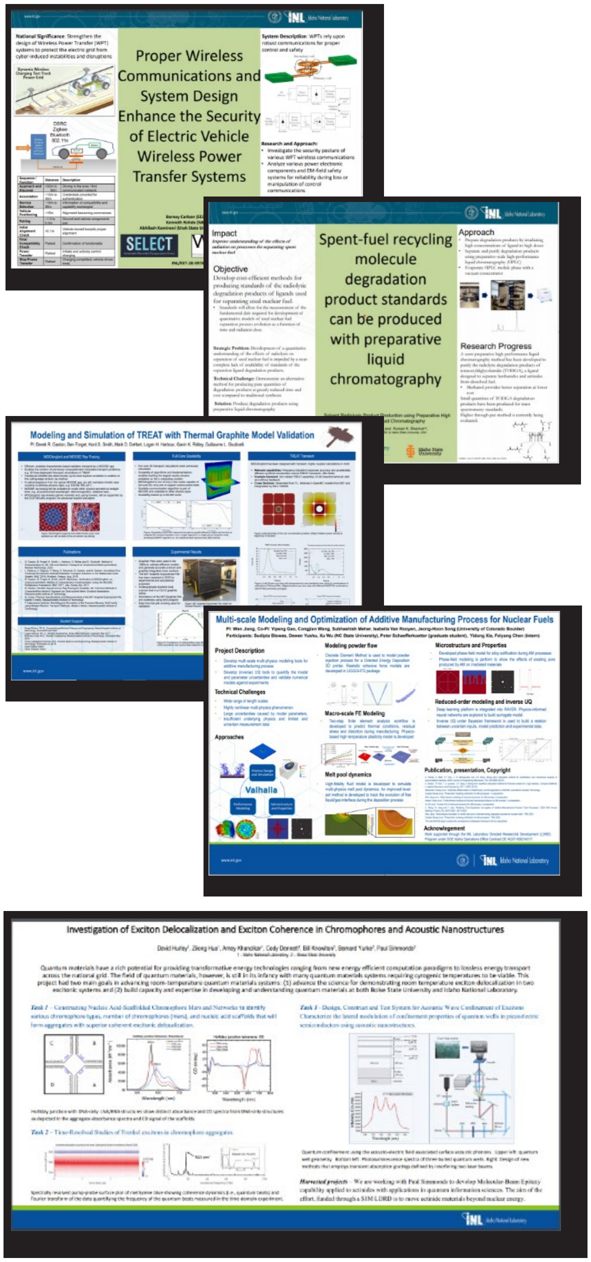
Core Capabilities

Of the 24 core capabilities distributed across DOE's science and applied-energy laboratories, INL has 13 DOE-acknowledged core and two emerging capabilities. The acknowledgement of these capabilities highlights the exceptional breadth of INL's scientific and technological foundation. The core capabilities represent a science and engineering skill set extending across a continuum, connecting basic and applied research to testing, demonstration, and deployment. These core capabilities are sustained and enhanced through INL's LDRD projects.

Project Selection & Oversight

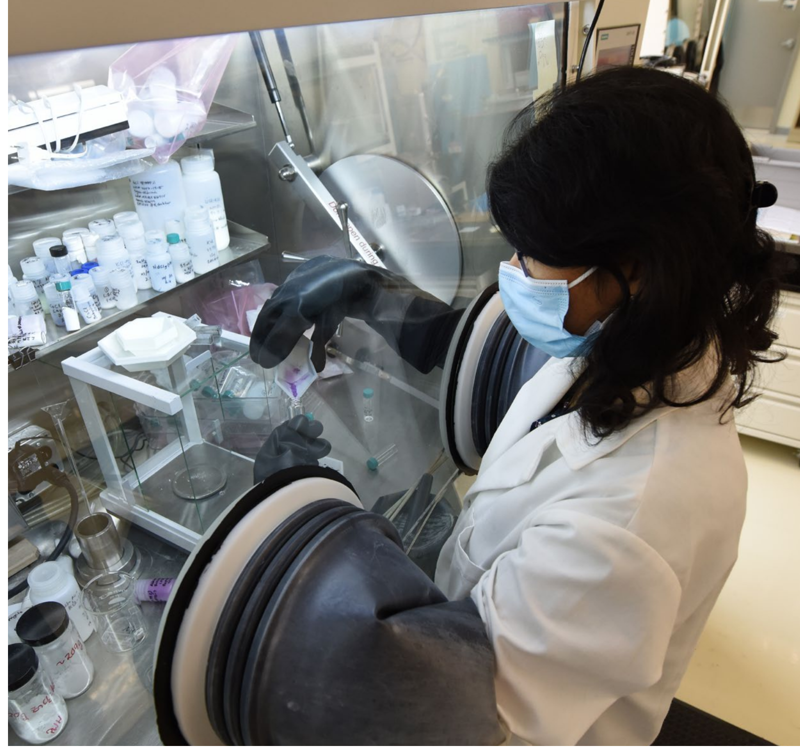
INL ensures that LDRD program goals and objectives are aligned with DOE Order 413.2C, Chg. 1, and that the LDRD portfolio is managed with integrity and transparency. New project proposals and project progress reports are subject to multiple levels of rigorous review by management and senior leadership. Lab leadership establishes review committees for each S&T initiative or investment area. These committees, staffed by senior and mid-career researchers and technical managers who are subject matter experts, review proposals and make recommendations on project selection. The deputy laboratory director for S&T reviews the committees' recommendations with the associate Laboratory directors and makes final funding decisions on the LDRD portfolio. Finally, Department of Energy Idaho Operations Office (DOE-ID) concurrence is requested on each proposal prior to project authorization.





FY 20 LDRD Poster Session

On September 24, 2020, INL hosted a virtual poster session showcasing 42 LDRD projects ending in FY 20. The virtual poster session mimicked traditional poster session interactions by facilitating chat access to principal and co-investigators and by providing all principal investigators with a presentation slot. Attendees included INL researchers, industry and academic partners, external collaborators, and members of the public.

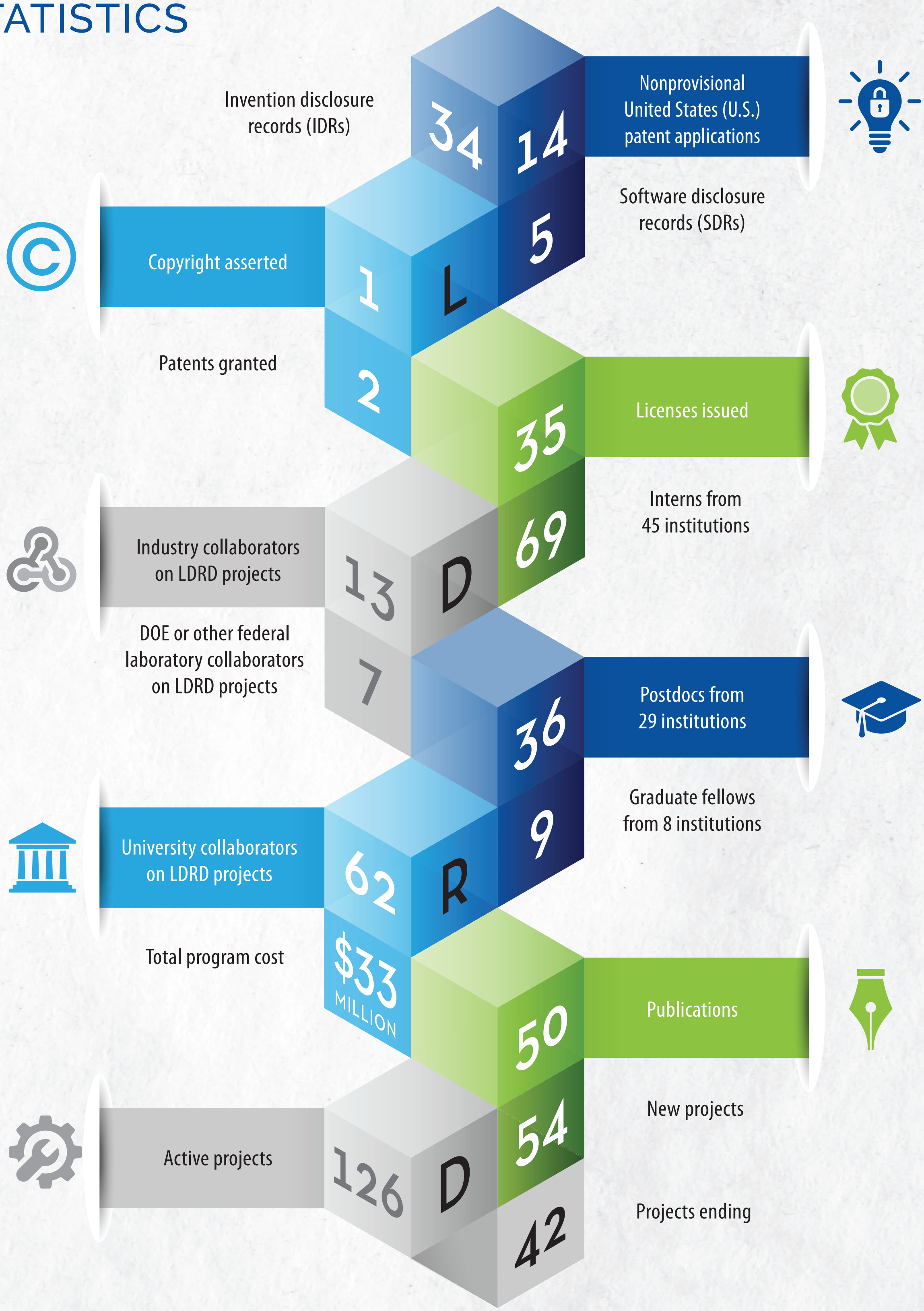


Distinguished Postdoctoral Researcher Program Attracts and Develops Early Career Researchers

INL has three named distinguished postdoctoral fellowships, all supported through LDRD: 1) Russell L. Heath Distinguished Postdoctoral Fellowship, 2) Deslonde de Boisblanc Distinguished Postdoctoral Fellowship, and 3) Glenn T. Seaborg Distinguished Postdoctoral Fellowship. The INL Distinguished Postdoctoral Researcher Program is designed to attract, recruit, develop and inspire early career researchers who have the potential to develop into INL's future scientific and technical leaders. These appointments are highly competitive and are intended to recognize and provide distinguished postdoctoral researchers with a competitive award, research experience, mentorship, and training to develop their capabilities. LDRD investments support the cutting-edge work of the next generation of INL's innovative workforce.

Abdalla Abou-Jaoude originally joined INL through the Distinguished Postdoctoral Researcher Program and has since converted to research staff. His LDRD project, "Feasibility Assessment of a Molten Salt Loop in the ATR," was part of the FY 18 Distinguished Postdoc Call.

FY 2020 PROGRAM STATISTICS



LDRD projects continue to advance the capabilities of INL's unique facilities such as ATR and TREAT.

NUCLEAR REACTOR SUSTAINMENT AND EXPANDED DEPLOYMENT

As DOE's nuclear energy laboratory, INL develops and demonstrates technology breakthroughs, technical solutions, and capabilities that will substantially improve the performance of existing and future nuclear energy systems and expand the use of nuclear systems. INL has a proven record as the leader in technological and operational advances, establishes and leverages national and international partnerships, and deploys world-class infrastructure to advance U.S. global competitiveness in existing and developing nuclear technology markets. The nuclear reactor sustainment and expanded deployment S&T initiative contributes to the development of a timely and cost-effective path to licensing and commercializing the next generation of nuclear energy systems and will enable the United States to regain and sustain leadership in advanced reactor technologies.

Enhance Testing and Experimentation Capabilities

INL is America's lead nuclear lab and sustains world-class nuclear energy RD&D capabilities on its 890-square mile site. These capabilities leverage INL's unique infrastructure including ATR, the Materials & Fuels Complex (MFC), and TREAT. Through LDRD, researchers steward and expand INL's experimental capabilities increasing the Lab's ability to execute advanced nuclear energy research. This year, LDRD investments continued to grow INL capabilities. For example, a project demonstrated the feasibility of a salt irradiation loop in the ATR, laying the groundwork for next-generation irradiation testing at ATR.[2] Another project developed an efficient tool for high-fidelity reactor analysis to reliably and predictively simulate both TREAT and the experiments placed within it.[3]

2 Project number 18P38-004: "Feasibility Assessment of a Molten Salt Loop in the Advanced Test Reactor"

3 Project number 18A12-206: "Modeling and Simulation of TREAT with Thermal Graphite Model Validation"

Feasibility Assessment of a Molten Salt Loop in the ATR

TOTAL APPROVED AMOUNT:
$257,000 over 3 years

PROJECT NUMBER:
18P38-004

PRINCIPAL INVESTIGATOR:
Abdalla Abou-Jaoude, INL
Deslonde de Boisblanc Distinguished Postdoctoral Researcher

CO-INVESTIGATORS:
Pattrick Calderoni, INL
James Sterbentz, INL

COLLABORATOR:
Boise State University

This project will enable the development and deployment of advanced reactors by demonstrating the feasibility of testing and qualifying materials using salt irradiation capabilities in existing facilities.

Molten salt reactors (MSRs) have garnered significant interest from industry and are getting ever closer to deployment. With more than eight U.S. companies pursuing salt-based reactor designs, the performance of previously untested salts will need to be evaluated prior to securing Nuclear Regulatory Commission (NRC) approval. This project conducted a feasibility study of a molten salt irradiation experiment inside ATR at INL as a potential solution to industry's need for testing capabilities. After reviewing the status of MSR technology, as well as the components needed for a salt loop experiment, a neutronic and thermal feasibility assessment demonstrated the suitability of different ATR positions to test various salt compositions. A preliminary design was developed, and natural circulation flow was simulated within a proposed setup. Initial engineering evaluations were conducted to ensure the feasibility of such an innovative and unique capability at ATR resulting in a conceptual design of the experiment dubbed the Versatile Experimental Salt Irradiation Loop (VESIL). By demonstrating the feasibility of a salt irradiation loop in the ATR, this project lays the groundwork for next-generation irradiation testing.

TALENT PIPELINE:

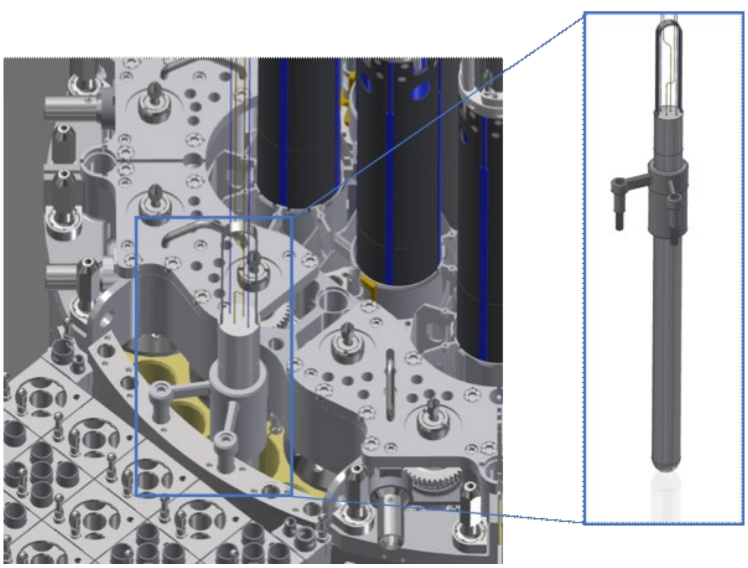
Students:

- Sandesh Bhaskar, North Carolina State University
- Samuel Walker, Rensselaer Polytechnic Institute

PRESENTATIONS:

Abou-Jaoude, A., S. Bhaskar, and C. Downey. 2020. "Conceptual Design of the Versatile Experimental Salt Irradiation Loop (VESIL) in the Advanced Test Reactor." Transactions of the American Nuclear Society 122, no. 1 (Virtual Conference June 8-11): 213-215. https://dx.doi.org/10.13182/T122-32438.

Bhaskar, S., and A. Abou-Jaoude. 2019. "Preliminary Design Evaluation of a Natural Circulation Molten Salt Irradiation Loop." Transactions of the American Nuclear Society 121, no. 1 (Washington, D.C., November 17-21): 1895-1896. https://dx.doi.org/10.13182/T30882.



A computer aided design illustration of the VESIL experiment assembly inside the ATR.

Development of Structural Elements in the Multiphysics Object-oriented Simulation Environment (MOOSE) Framework

TOTAL APPROVED AMOUNT:
$578,600 over 3 years

PROJECT NUMBER:
18A12-201

PRINCIPAL INVESTIGATOR:
Albert Casagranda, INL

CO-INVESTIGATORS:
Justin Coleman, INL
Benjamin Spencer, INL

Researchers developed new capabilities to simulate structural elements targeting two problems of interest to the nuclear industry: seismic analysis of nuclear power plant structures and modeling of fuel assemblies.

Prior to this project, the INL-developed MOOSE framework was limited to modeling structures using continuum (brick) elements. Continuum elements provide great flexibility for modeling a variety of geometries but can be impractical for modeling components that are very thin in one or more directions such as nuclear fuel assemblies, containment structures, and structural components including beams, columns, walls, and floor panels. Addressing this gap targeted two problems of interest to the nuclear industry: seismic analysis of nuclear power plant structures and modeling of fuel assemblies. Beam and shell elements are well suited to capture the bending/flexure deformations experienced by the very thin components that can be found in nuclear fuel assemblies and other nuclear power plant components. This project developed new capabilities for MOOSE including beam and shell elements, lumped mass models, and tools for extracting quantities useful in American Society of Mechanical Engineers code analyses targeting seismic analysis of nuclear power plant structures and modeling of fuel assemblies. These capabilities are complementary to the existing unique capabilities in applications based on MOOSE and improved their ability to be used in engineering design and safety analyses. The increased structural mechanics capabilities developed though this project expand the range of problems that can be solved using MOOSE and MOOSE-based applications.

TALENT PIPELINE:

Student:

- Hrishiv Neupane, University of Utah

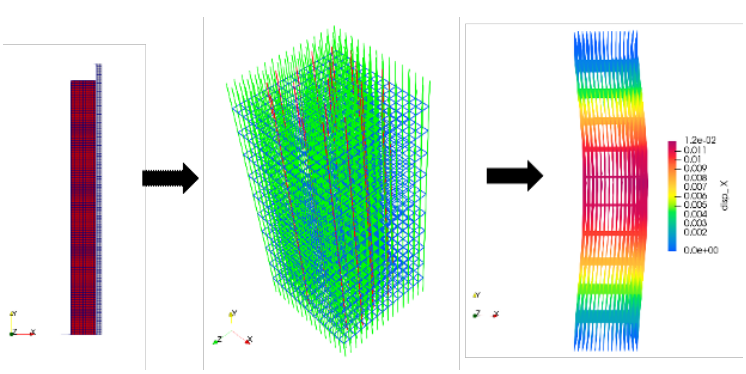
PUBLICATION:

Veeraraghavan, S., C. Bolisetti, A. Slaugher, J. Coleman, S. Dhulipala, W. Hoffman, K. Kim, E. Kurt, R. Spears, and L. Munday. 2020. "MASTODON: An Open-Source Software for Seismic Analysis and Risk Assessment of Critical Infrastructure." Nuclear Technology (Oct.). https://doi.org/10.1080/00295450.2020.1807282.

PRESENTATIONS:

Veeraraghavan, S., A. Casagranda, and B. Spencer. 2019. "Modeling Fuel Assembly Distortion in Light Water Reactors Using BISON." Presented at the TopFuel 2019 Light Water Reactor Fuel Performance Conference (Seattle, WA, Sept. 22-26).

Veeraraghavan, S., and J. Coleman. 2019. "Effect of Non-vertically Propagating Earthquake Waves and Nonlinear Soil-structure Interaction on Nuclear Facility Response," Transactions of the 25th International Conference in Structural Mechanics in Reactor Technology (Charlotte, NC, Aug. 4-9). https://www.lib.ncsu.edu/resolver/1840.20/37657.



The fuel assembly distortion model combines two-dimensional (2D) axisymmetric models for each rod in a 16x16 assembly with the full assembly modeled with beam elements to show the bowing of a pressurized water reactor fuel assembly as a result of spatially asymmetric power profiles (displacements and axial direction scaled for clarity).

Realizing Multidimensional Imaging and Machine Learning on the Scanning Transmission Electron Microscope

TOTAL APPROVED AMOUNT:
$897,100 over 3 years

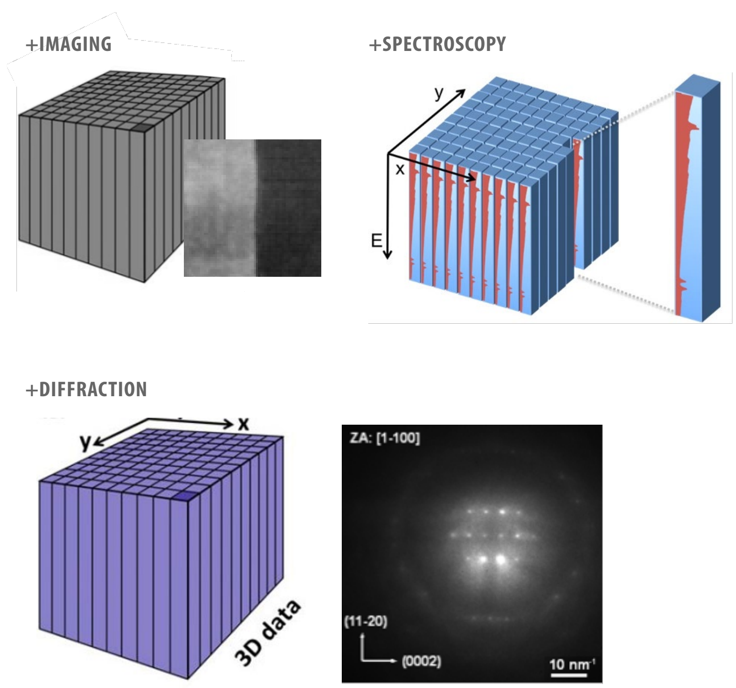
PROJECT NUMBER:
18A12-029

PRINCIPAL INVESTIGATOR:
Jeffery Aguiar, formerly INL

CO-INVESTIGATORS:
John Bradley, University of Hawai'i at Mānoa
Nigel Browning, University of Liverpool
Ricardo Castro, University of California Davis
Peter Crozier, Arizona State University
Matthew Gong, University of Utah
Ross Kunz, INL
Benjamin Miller, Gatan, Inc.
Brandon Miller, INL
Bryan Reed, Integrated Dynamic Electron Solutions
Michael Scarpulla, University of Utah
Tolga Tasdizen, University of Utah
Jess Tate, University of Utah
Raymond Unocic, Oak Ridge National Laboratory (ORNL)

An automation and high-throughput framework for simultaneous imaging, diffraction, and spectroscopy inside a scanning transmission electron microscope (STEM) to assemble quantitative and deconstruct multidimensional datasets was developed using INL instrumentation and expert collaborators.

Transmission electron microscopy (TEM) is a tool for detailed structural and chemical analysis, extending from the micron to the atomic scale. However, simultaneous data collection in the latest generation of STEMs is restricted by current software and hardware, forcing researchers to use multiple tools and methods to collect and analyze data, which increases cost and reduces efficiency. INL researchers identified an opportunity for the development of simultaneous modes of operation with improved spatial and temporal fidelity for scanning transmission electron microscopes. A growing percentage of cutting-edge R&D now utilizes STEM-based X-ray spectroscopy to provide weighted elemental maps at the atomic or higher size scales to inform material processes and growth. Alternatively, diffraction-based imaging is the only accepted crystallography-based technique for resolving structure-related information. Due to the limited spatial resolution of diffraction-based imaging, studying atomic defects and interfaces with diffraction has not been considered correlative with high-resolution STEM; however, recent efforts have shown that the newest electron microscopes may have the capability. Researchers found that the development of simultaneous modes of operation and collection helps reduce delays in data access, extraction, and costs. This research provides a clear technical method for early adoption within numerous scientific and engineering communities.



Multimodal data assembly and manipulation developed in this effort enables increased breadth of input data and near automated classification of electron microscopy.

INTELLECTUAL PROPERTY:
One software copyright filed (CW-20-26): Technique for Extrapolating Particle Compaction Profiles from Collected X-ray Tomography Datasets

PUBLICATIONS:
Aguiar, J.A., M.L. Gong, T. Tasdizen, and B.D. Miller. 2020. "Crystallographic Prediction from Diffraction and Chemistry Data for Higher Throughput Classification Using Machine Learning." Computational Materials Science 173: 109409. https://doi.org/10.1016/j.commatsci.2019.109409.

Aguiar, J.A., M.L. Gong, R.R. Unocic, T. Tasdizen, and B. Miller, B.D. 2019. "Decoding Crystallography from High-Resolution Electron Imaging and Diffraction Datasets with Deep Learning." Science Advances 5, no. 10 (Oct.): eaaw1949. https://doi.org/10.1126/sciadv.aaw1949.

Machine Learning Helps Scientists Interpret Crystal Patterns

For scientists and engineers, the best way to understand a new or unknown material—whether it's an alloy, a pharmaceutical or a meteorite—is to delve into its atoms.

Techniques such as X-ray diffraction, microscopy, and spectroscopy can give insights into a material's crystal orientation, structure, and chemical composition, information that's often vital for predicting the performance of advanced materials such as nuclear fuels.

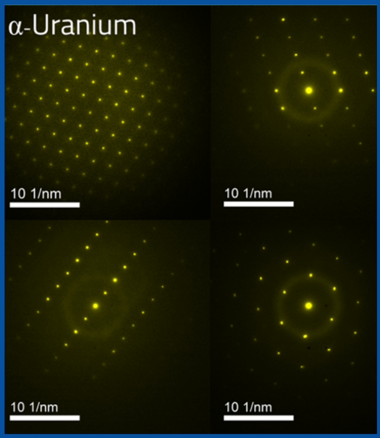
However, analyzing data from these methods, especially diffraction patterns, is a time-consuming process.

Now, Idaho National Laboratory researchers have helped develop a computer model that can interpret diffraction patterns in hours instead of weeks. The research appears in the journal Science Advances.

A diffraction pattern is the result of a beam of light, X-rays, neutrons or electrons scattering off a well-ordered or amorphous crystalline material. The crystals bend the beam into a particular pattern that is projected onto a camera sensor or photographic paper. Interpreting the patterns provides a knowledge of the underlying material structure down to the local arrangement of atoms.

Until now, interpreting those raw, experimental images was difficult, said INL staff scientist Jeff Aguiar.

"Everyone's asking, 'What's the crystal structure?' and 'What's the coordination of the atoms?' It's pretty daunting for people," he said. "They take out modern versions of a protractor and a ruler and open the Standard X-ray Diffraction Powder Patterns handbook."



The model has been evaluated on materials with a range of symmetries. This image shows the diffraction pattern of a less symmetrical material: orthorhombic α-phase uranium.

A Daunting Task Made Easier

Even with the tools and the know-how, using the current methods to analyze diffraction patterns of complex materials can take months. To prove this point, Aguiar and his colleagues sent a challenging series of diffraction patterns to experts across the country.

"We made a Google survey and sent it out to national lab folks, university professors, and graduate students and asked them what the structure is," he said. "It took anywhere from a week to six months. The individual who was the most accurate took six months."

The new INL model came from a desire to streamline this laborious process from weeks or months to a few hours. "It's using the data that's out there to push the community forward from the routine analysis that we've all struggled with since grad school," Aguiar said.

https://inl.gov/article/machine-learning-for-crystal-patterns/

The Influence of Irradiation on the Corrosion Kinetics and Hydrogen Pickup of Zirconium Alloys

TOTAL APPROVED AMOUNT:
$725,400 over 3 years

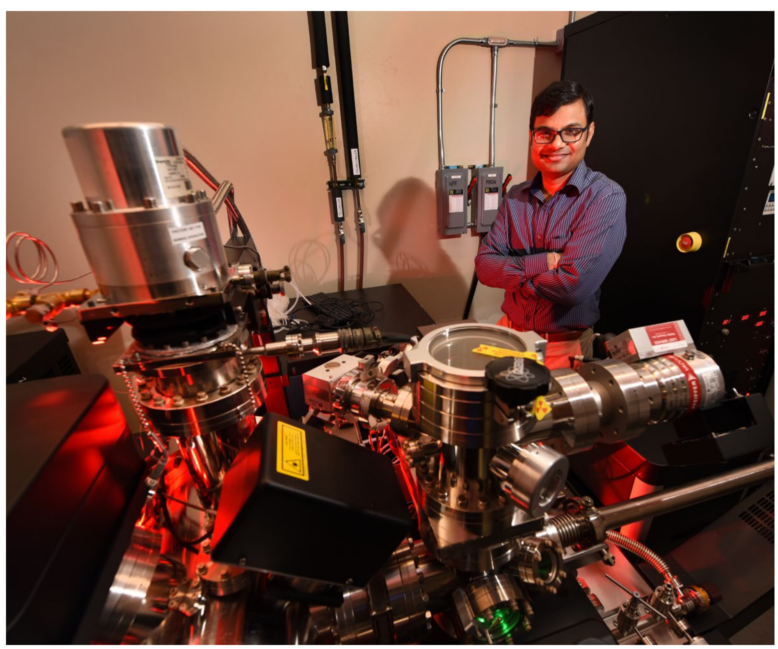
PROJECT NUMBER:
17P11-014

PRINCIPAL INVESTIGATOR:
Mukesh Bachhav, INL

CO-INVESTIGATORS:
Joshua Bowman, Pennsylvania State University
Jesse Carter, Navy Nuclear Laboratory
Adrien Couet, University of Wisconsin
Daniel Jädernäs, Studsvik, Swedish Operations
Bruce Kammenzind, Navy Nuclear Laboratory
Arthur Motta, Pennsylvania State University
Richard Smith, Navy Nuclear Laboratory
Peng Wang, University of Michigan
Gary Was, University of Michigan
Zefeng Yu, University of Wisconsin

Researchers explored the mechanisms governing oxidation and hydriding under irradiation in the reactor environment to improve the performance of zirconium alloys in light water reactors.

One of the critical challenges for the nuclear industry is to understand the evolution of the properties of zirconium alloys during irradiation and the effect of these changes on corrosion behavior. The primary factor limiting the utilization of fuel rods is waterside corrosion and the resulting hydrogen pickup. As a result of oxidation and hydrogen pickup, hydrides form and accumulate in cladding, causing embrittlement and limiting fuel lifetime. Because the factors that affect corrosion and hydriding are complex and can be interdependent, separate effects testing was implemented to obtain a more fundamental understanding of these behaviors. Researchers used a combination of ion irradiation, autoclave exposure, and advanced characterization techniques to study the effect of irradiation on the corrosion kinetics of zirconium alloys. Ion irradiation has been shown to replicate the basic features of in-reactor irradiation that appear to most strongly affect corrosion behavior, including amorphization and dissolution of precipitates and second phase particles in Zircaloy-4. This research focused on emulating irradiation effects caused by neutrons in reactor condition using protons and heavy ions. The data generated contributes to the development and validation of models to better understand the oxidation and hydrogen pickup mechanisms in zirconium-based alloys with potential implications for issues affecting fuel such as loss-of-coolant accidents, reactivity-initiated accidents, channel and fuel assembly distortion, hydrogen embrittlement and cracking, seismic performance, secondary fuel degradation, and dry cask storage and transportation.



Advanced characterization techniques were used to study the microstructure of the of Zircaloy-4 to understand microstructural changes caused by irradiation.

TALENT PIPELINE:

Student:

- Evrard Lacroix, Pennsylvania State University

PUBLICATIONS:

Yu, Z., A. Couet, and M. Bachhav. 2019. "Irradiation-induced Nb Redistribution of ZrNb Alloy: An APT Study." Journal of Nuclear Materials, 516, no.1 (April): 100-110. https://doi.org/10.1016/j.jnucmat.2019.01.015.

Yu, Z., T. Kim, M. Bachhav, X. Liu, L. He, and A. Couet. 2020. "Effect of Proton Pre-irradiation on Corrosion of Zr-0.5Nb Model Alloy with Different Nb Distribution." Corrosion Science (June): 108790. https://doi.org/10.1016/j.corsci.2020.108790.

PRESENTATION:

Yu, Z. M. Bachhav, L. He, A. Couet. 2020. "TEM and APT Characterization of Neutron Irradiated AXIOM- 2(X2)®." Transactions of the American Nuclear Society 123, (Virtual Winter Meeting Nov. 16-19): 599-602. https://doi.org/10.13182/T123-33175.

Growing the Next Generation of Scientists and Engineers

LDRD investments allow INL to directly feed the talent pipeline by exposing students to hands-on laboratory experience and the opportunity to work with world-class personnel. The work on this LDRD project formed the basis for one master's thesis:

Bowman, J. 2020. "Transmission Electron Microscopy Characterization." Master's thesis. Pennsylvania State University.

INL's CAES is a research and education consortium among INL, Boise State University, Idaho State University, the University of Idaho, and the University of Wyoming. CAES is a connected research environment providing researchers with seamless virtual and physical access to state-of-the-art facilities and laboratories.

An Advanced Reactor Fuel Performance Tool Based on Coupled BISON and Monte Carlo Simulation Using MOOSE

TOTAL APPROVED AMOUNT:
$715,600 over 3 years

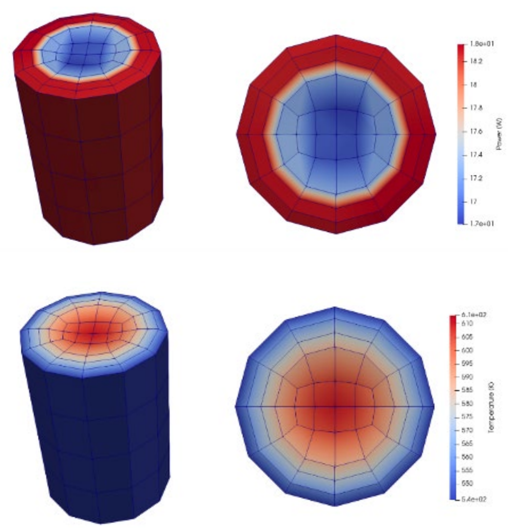
PROJECT NUMBER:
18A12-178

PRINCIPAL INVESTIGATOR:
Mark DeHart, INL

Researchers leveraged INL's MOOSE and MOOSE-wrapped application technology to couple the fuel performance code BISON to an advanced radiation transport code.

Both deterministic and Monte Carlo methods for neutron transport have limitations and strengths for reactor analysis. Due to the wider availability of affordable large-scale computing platforms, there is growing interest in the use of Monte Carlo methods for reactor design calculations that are currently performed using few-group diffusion theory or other low-order methods. Researchers coupled a Monte Carlo simulation to MOOSE tools using MOOSE and MOOSE-wrapped application technology to pair BISON to an advanced radiation transport code. Using the power distribution provided by Monte Carlo solutions through the Pipistrelle MOOSE-wrapped app, this research was able to communicate result direction to BISON, which was then used to compute a temperature distribution that is transferred to Pipistrelle as output. Pipistrelle writes an updated input file and restarts the Monte Carlo code. This research demonstrates the potential for coupling Monte Carlo-based radiation transport simulations with MOOSE-based tools using the MOOSE-wrapped application approach.

TALENT PIPELINE:
Student:
- Zachary Hills, Oregon State University



Power density extracted from the Monte Carlo solver and mapped to the finite element mesh (top) and temperature distribution from BISON solution using the power density provided (bottom).

Development of a Quantitative Measurement Technique for Fission Gas Bubble Pressure at Nanoscale Using Advanced Characterization and Modeling Techniques

TOTAL APPROVED AMOUNT:
$133,400 over 1 year

PROJECT NUMBER:
19A42-017

PRINCIPAL INVESTIGATOR:
Lingfeng He, INL

CO-INVESTIGATORS:
Larry Aagesen, INL
Jian-Min Zuo, University of Illinois at Urbana-Champaign

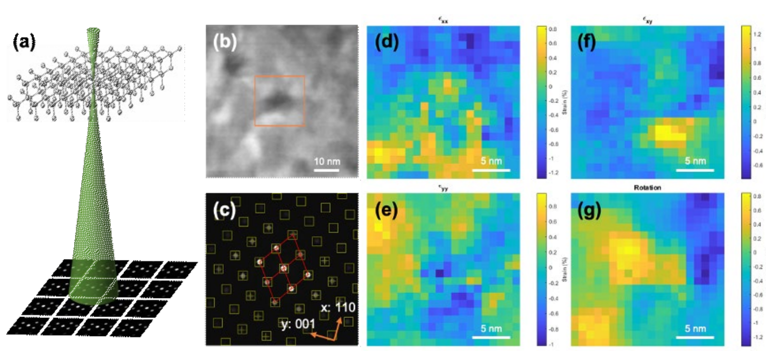
Researchers developed a scanning electron nanodiffraction (SEND) capability to quantitatively measure fission gas bubbles from microscale to nanoscale to better understand the behavior of nuclear reactor fuels after irradiation.

Quantitative measurements need to be done at the length scale of the feature to better understand the behavior of nuclear reactor fuel materials after irradiation. Current methods either do not provide enough spatial resolution or lack sensitivity. This project introduced a new characterization technique, SEND, to study nuclear materials at nanoscale. Using advanced methods to analyze the four-dimensional (4D) datasets from SEND, researchers measured the strain fields around fission gas bubbles at multiple orientations. A machine learning approach was used to obtain high resolution orientation maps of low-angle grain boundaries due to grain subdivision. The strain field surrounding an underpressurized gas bubble was also calculated using a phase-field model that accounts for the gas pressure and surface tension. The combination of the SEND technique plus machine learning advances INL's material characterization capabilities and has applications to understanding the strength of bonding in welded parts and of duel and multi-phase materials used in reactor applications.

TALENT PIPELINE:
Student:
- Renliang Yuan, University of Illinois at Urbana-Champaign

PUBLICATION:
Renliang, Y., J. Zhang, L. He, and J.-M., Zuo. 2021. Training Artificial Neural Networks for Precision Orientation and Strain Mapping Using 4D Electron Diffraction Datasets. Ultramicroscopy, 113256 (Mar.). https://doi.org/10.1016/j.ultramic.2021.113256.

PRESENTATION:
He, L., M. Bachhav, C. Jiang, D. Sprouster, D. Shuh, B. Miller, L. Ecker, and J. Gan. 2019 "Advanced Characterization of Fission Products in Nuclear Fuels." Invited presentation at the American Chemical Society Fall 2019 National Meeting & Exposition (San Diego, CA. Aug. 25-29).



(a) Schematic of SEND. (b) High-angular annular dark-field image of xenon bubble. Orange box indicates the scanning area for SEND data acquisition. (c) An example diffraction pattern in the SEND dataset used for strain measurement. Diffraction disks are detected using circular Hough transform. (d-g) Strain maps of uranium dioxide matrix containing a xenon bubble.

Coupled Multiphysics Simulation of Seismic Response of Degraded Concrete Dams

TOTAL APPROVED AMOUNT:
$78,000 over 1 year

PROJECT NUMBER:
20A1047-013

PRINCIPAL INVESTIGATOR:
Chandrakanth Bolisetti, INL

CO-INVESTIGATOR:
Benjamin Spencer, INL

Researchers studied the impact of alkali-silica reaction (ASR), a common degradation mechanism in aging concrete structures, to assess seismic and other external hazard risk in aging structures, such as dams and nuclear power plants.

Concrete degradation from ASR can result in a loss of strength and stiffness leaving concrete structures potentially more vulnerable to external hazards such as earthquakes. For example, ASR has caused cracking in several below-grade structures at the Seabrook Nuclear Power Plant and in dams and bridges across the United States. As a part of this work, researchers coupled two MOOSE based software applications, Multi-hazard Analysis for STOchastic time-DOmaiN phenomena (MASTODON), a seismic analysis and risk assessment software, and BlackBear, a concrete and other structural material degradation analysis software and created a novel, unified capability that greatly simplifies the seismic analysis of aging structures. Researchers demonstrated that the combined code can successfully be used for performing fully coupled simulations of ASR-degraded dams subjected to earthquakes, while including the earthquake fault-rupture-to-site wave propagation. Researchers also performed aging simulations of the Seminoe dam in Wyoming and showed that the newly developed code can reproduce ASR-related deformation trends in the dam that have been observed over the years in the field. This research creates and demonstrates a software tool that improves performance of seismic and other external hazard assessments of aging concrete structures like dams and nuclear power plants.

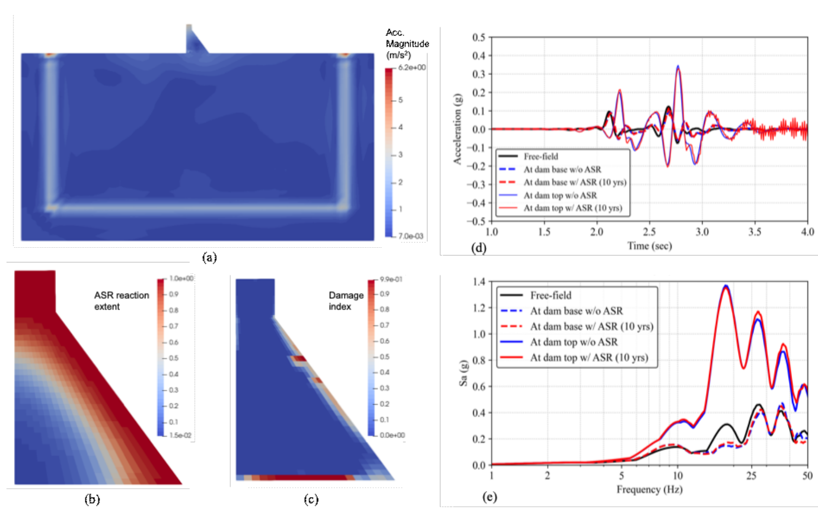
TALENT PIPELINE:

Postdoc:

- Kyung Tae Kim, INL

PRESENTATION:

Kim, K., B. Spencer, and C. Bolisetti. 2020. "Coupled Multiphysics Simulations of Seismic Response of Degraded Concrete Structures." Presented at the DOE/NRC Natural Phenomena Hazards Meeting (Virtual Meeting, Oct. 20-22). https://www.nrc.gov/docs/ML2028/ML20280A450.pdf.



Simulation results from the earthquake fault rupture scenario: (a) contour of acceleration magnitude at 2.8 sec in the region of interest as peak structure acceleration occurred; (b) ASR extent prior to seismic shaking; (c) damage index at the end of seismic shaking; (d) acceleration histories and (e) 2% damped acceleration response spectra at free-field (in the absence of the dam), and at the top and the base of the dam with and without considering 10-year ASR deterioration.

Implementation of Novel Analytical Procedures for Quantification of Fission Products and Impurities in Nuclear Fuels Using a High Resolution Inductively Coupled Plasma Mass Spectrometer (HR-ICP-MS)

TOTAL APPROVED AMOUNT:
$131,100 over 1 year

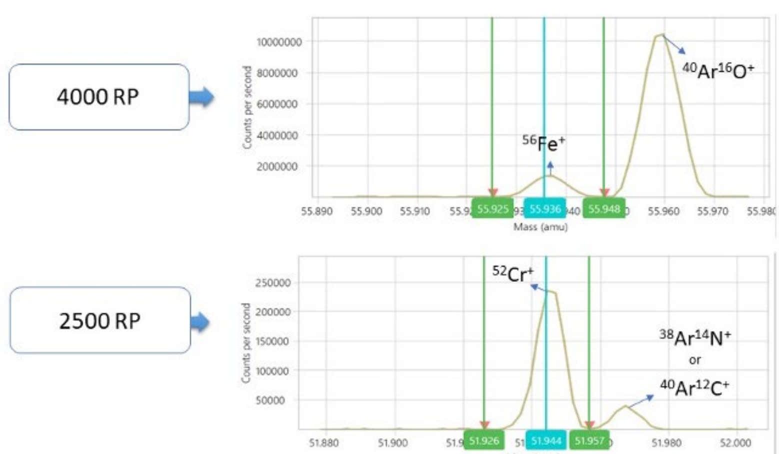
PROJECT NUMBER:
19A1045-017

PRINCIPAL INVESTIGATOR:
Vivian Montes de Oca Carioni, INL

CO-INVESTIGATORS:
Beau Barker, INL
Luiza Gimenes Rodrigues
Albuquerque, INL

Researchers developed and implemented a new procedure to attach a HR-ICP-MS to a radiological hood that reduces or eliminates the interferences in the analysis of nuclear fuels and reactor components while maintaining high instrumental sensitivity.

The development of advanced reactors has moved toward a more comprehensive characterization of fuel and reactor components. The availability of accurate, highly sensitive, and high throughput analytical characterization of nuclear fuel materials is a critical step in the development of next-generation nuclear reactor fuels. Most of the characterization is currently performed using quadrupole ICP-MS. However, a major disadvantage of ICP-MS is the formation of interfering species due to the the recombination of ions from the plasma gas, acids, or solvents. These unwanted species have nearly the same mass-to-charge ratio as the species of interest, which results in increased background signal and false positives. The novel analytical method developed in this project mitigates these problematic interferences. The advantage of the HR-ICP-MS instrument is that it has a high resolving power of >10,000; a high enough resolving power to separate potential interferences from analytes. Different mass interferences require different resolving powers to be separated from analytes, and this can become complex depending on the sample composition. The trade-off between resolution and instrumental quantification limits was also evaluated in this study. Although using a higher resolving power decreases the instrumental sensitivity in some instances, the elimination of the background signal due to a mass interference had a positive effect on the instrumental quantification limit. Considering the low- and high-resolution methods, the instrumental quantification limits could be improved by factors up to 100 when compared with the quadrupole inductively coupled plasma mass spectrometry. The availability of accurate and highly sensitive analytical characterization methods developed for the analysis of as built and post-irradiated fuels using the new HR-ICP-MS results in more reliable determination of isotopes in complex nuclear samples contributing to the development of next-generation nuclear reactor fuels.



Separation of $^{56}Fe^+$ from $^{40}Ar^{16}O^+$ by HR-ICP-MS in 4,000 resolving power and separation of $^{52}Cr^+$ from $^{38}Ar^{14}N^+$ or $^{40}Ar^{12}C^+$ by HR-ICP-MS in 2,500 resolving power.

Modeling and Simulation of TREAT with Thermal Graphite Model Validation

TOTAL APPROVED AMOUNT:
$842,400 over 3 years

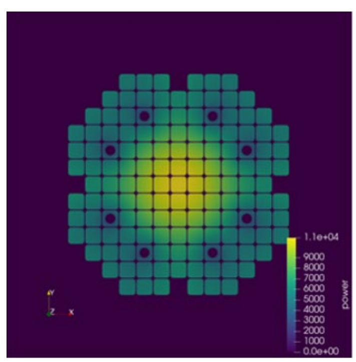
PROJECT NUMBER:
18A12-206

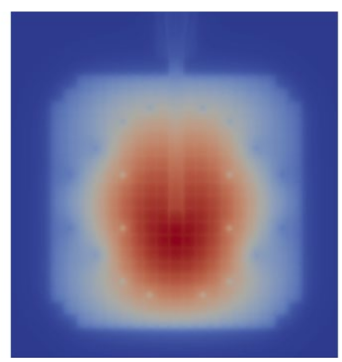
PRINCIPAL INVESTIGATOR:
Derek Gaston, INL

CO-INVESTIGATORS:
Mark DeHart, INL
Benoit Forget, MIT
Jean Ragusa, Texas A&M University
Kord Smith, MIT

Researchers focused on the modeling and simulation of TREAT, which produces transient pulses that can be tailored for the application. This is a challenging problem requiring a special multiphysics-capable reactor analysis tool combined with a science-based approach for verification, validation, and nuclear data generation.

Following INL's successful restart of TREAT in 2017, it became clear that a large component of future operations in the reactor depended on reliable modeling and simulation. The same characteristics that make TREAT a unique, world-leading nuclear test bed also pose challenges for modeling and simulation: it is inherently transient; it has inter-element air gaps and is often used with a hodoscope slot, providing long streaming paths for neutrons; it is known to have poorly characterized fuel material characteristics; it has strong thermal feedback; and it has an uncommon geometry compared to operating light-water reactors. In this project, researchers leveraged the unique characteristics of the newly developed MOOSE-based reactor analysis tool MOCkingbird, using the method of characteristics (MOC), to develop a high-fidelity simulation of radiation transport in the TREAT reactor. Additional verification, validation, and nuclear data generation was provided through collaboration with the Massachusetts Institute of Technology (MIT) on their instrumented graphite pile. Novel computational algorithms for massively parallel ray tracing, mesh partitioning, mesh adaptivity, mesh generation, and sparse parallel communication capabilities resulting from this research have gone into MOOSE, accelerating an extensive range of diverse applications reaching far beyond this project's purview for years to come. The MOCkingbird tool has been verified against several benchmarks, including a first-of-a-kind, full-core, three-dimensional (3D) solution of the Benchmark for Evaluation and Validation of Reactor Simulations and TREAT benchmarks. MOCkingbird enables accurate and efficient high-fidelity reactor analysis by reliably and predictively simulating both TREAT and the experiments placed within it.





TREAT minimum critical mass power distribution with rods in (left) and TREAT M8 calibration series configuration fast flux with transient rod bank in with streaming effects seen in the hodoscope (right).

TALENT PIPELINE:

Students:

- Logan Harbour, Texas A&M University
- Leora Chapuis, Polytech Lyon
- Travis Labossiere-Hickman, MIT
- Gavin Ridley, MIT
- Nicholas Costa, MIT
- Isaac Meyer, MIT

PUBLICATION:

Gaston, D., B. Forget, K. Smith, L. Harbour, G. Ridley, and G. Giudicelli. Accepted for publication in 2021. "Method of Characteristics for 3D, Full-core Neutron Transport on Unstructured Mesh." Nuclear Technology.

PRESENTATIONS:

Harbour, L., J. Ragusa, Y. Wang, S. Schunert, D. Gaston, and M. DeHart. 2019. "Uncollided-Flux Treatment for Discrete-Ordinate Radiation Transport Solutions in the Rattlesnake Code System." Presented at the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (Portland, OR, Aug.25-29).

Gaston, D., B. Forget, K. Smith, and R. Martineau. 2017. "Verification of MOCkingbird, an Unstructured- Mesh, Method of Characteristics Implementation Using the MOOSE Multiphysics Framework." Presented at the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (Jeju, Korea, Apr. 16-20).

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Gaston, D. 2020. "Parallel, Asynchronous Ray-Tracing for Scalable, 3D, Full-Core Method of Characteristics Neutron Transport on Unstructured Mesh." Ph.D diss., MIT.

Costa, N. 2020. "Physical Specifications and Measurements of the MIT Graphite Exponential Pile." Master's thesis. MIT. https://dspace.mit.edu/handle/1721.1/127302

Labossiere-Hickman, T. 2019. "Modeling and Simulation of the Transient Reactor Test Facility Using Modern Neutron Transport Methods." Master's thesis. MIT. https://dspace.mit.edu/handle/1721.1/123360

Harbour, L. 2017. "Uncollided Flux Implementation for Discrete Ordinates Radiation Transport Solutions in Rattlesnake." Master's thesis. Texas A&M University.

Small Scale Tensile Testing Technique for Measuring Grain Boundary Strength of Neutron-irradiated Materials in Focused Ion Beam Systems

TOTAL APPROVED AMOUNT:
$767,600 over 3 years

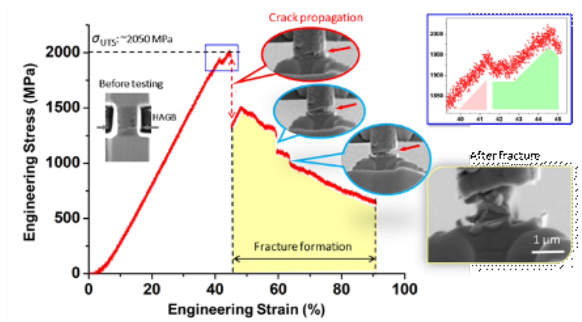
PROJECT NUMBER:
18A12-150

PRINCIPAL INVESTIGATOR:
Lingfeng He, INL

CO-INVESTIGATORS:
Mukesh Bachhav, INL
Xianming Bai, Virginia Polytechnic Institute and State University (Virginia Tech) and INL
Wen Jiang, INL
Jie Lian, Rensselaer Polytechnic Institute
Daniel Murray, INL
Cheng Sun, INL
Russell L. Heath Distinguished Postdoctoral Researcher

Researchers established the quantitative relationship between the strength and character/microchemistry for individual grain boundaries to better understand the material property changes influenced by microstructure evolution under extreme operating conditions.

Irradiation induced defects or microchemistry change like element segregation at grain boundaries can lead to the degradation of grain boundary strength and further cause intergranular cracking in structural materials, affecting the safe operation and service life of nuclear reactors. Establishing the quantitative relationship between the strength and character/microchemistry for individual grain boundaries by coupling experimental characterization and multiscale simulation allows for a better understanding of the material property changes influenced by microstructure evolution under extreme operating conditions. In this project, a novel methodology was developed for the fabrication of micro-tensile specimens with a grain boundary of interest and an *in situ* small-scale tensile testing method for the measurement of grain boundary strength in focused ion beam systems. Additional microchemistry investigation by a series of advanced characterization techniques provided key input information for the modeling of intergranular fracture in materials. Atomistic modeling was performed to calculate the cohesive strength of different grain boundaries and to explore how the segregation of substitutional solute and impurity elements affects embrittlement potency. This methodology enables rigorous study of grain boundary strength of alloys exposed in simultaneous corrosion / irradiation environments.



The engineering stress-strain curve for pristine X-750 micro-tensile specimen shows a crack propagated rapidly in a shallow surface layer on the gauge, showing brittleness followed by a fracture formation process dominated by more ductile deformation until complete fracture at the grain boundary, demonstrating that the X-750 alloy fractures in a mixture of brittle and ductile behavior.

TALENT PIPELINE:

Postdoc:

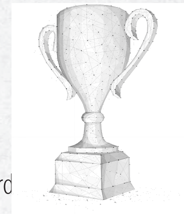
- Xiang Liu, INL

Students:

- Axel Seoane, Virginia Tech
- Ziqi Xiao, Virginia Tech
- Yaxuan Zhang, Virginia Tech
- Yachun Wang, Rensselaer Polytechnic Institute
- Pengyuan Xiu, University of Michigan

AWARDS:

- Xiang Liu, 2018 American Nuclear Society Mark Mills Award
- Xiang Liu, 2019 University of Illinois Ross Martin Award



PUBLICATION:

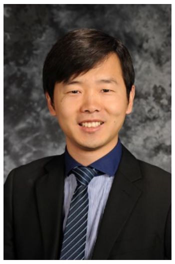
Liu, X., L. He, H. Yan, M.Bachhav, and J. F. Stubbis. 2020. "A Transmission Electron Microscopy Study of EBR-II Neutron-irradiated Austenitic Stainless Steel 304 and Nickel-base Alloy X-750." Journal of Nuclear Materials, 528 (Jan.): 151851. https://doi.org/10.1016/j.jnucmat.2019.151851.

PRESENTATIONS:

He, L., M. Bachhav, D. Murray, X. Liu, E. Perez, W. Jiang, Z.Xiao, X. Bai, C. Sun, and S. Teysseyre, 2019. "Effects of Element Segregation/Depletion and Precipitates on Grain Boundary Strength of Alloys." Invited presentation to the Minerals, Metals, & Materials Society 148th Annual Meeting & Exhibition (San Antonio, TX, March 10-14).

He, L., D. Murray, X. Liu, W. Jiang, M. Bachhav, X. Bai, and S. Teysseyre. 2019. "Small Scale Tensile Testing of Grain Boundary Strength of X-750 Alloy." Proceedings of the 19th International Conference on Environmental Degradation of Materials in Nuclear Power Systems-Water Reactors (Boston, MA, Aug. 11-15).

Xiang Liu came to INL as a postdoctoral researcher and converted to INL research staff in May 2020. Liu's work on this LDRD project earned him two research awards.



Dynamic Behavior of Nuclear Fuels in Hydrogen Coolant for Nuclear Thermal Propulsion (NTP) and Mitigation of Thallium-208 Gamma Dose from Plutonium-236 Decay via Chemical Removal of Uranium-232

TOTAL APPROVED AMOUNT:
$275,000 over less than 1 year

PROJECT NUMBER:
20A1051-001

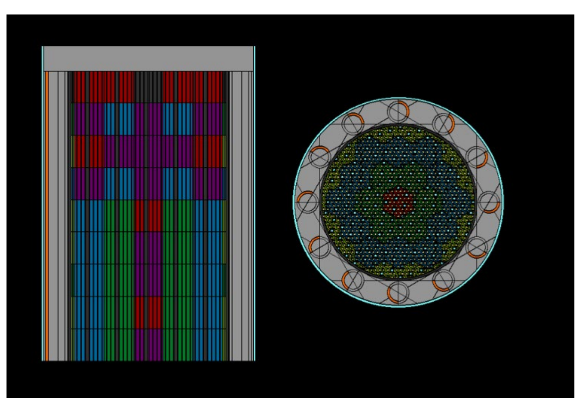
PRINCIPAL INVESTIGATOR:
Stephen Johnson, INL

CO-INVESTIGATORS:
Eric Clarke, INL
Brad Kirkwood, INL
Steve Herring, Center for Space Nuclear Research

Researchers addressed two problems concerning nuclear power in space: rapid shutdown thermal transients in nuclear thermal propulsion reactors, which can make fuel inefficient or even lead to fuel failure, and reduction of the occupational dose during assembly of plutonium-238 power generators through careful timing of the removal of uranium-232.

Future human exploration of Mars and the outer solar system will require the use of nuclear energy to reduce travel time and thus the exposure of the crew to energetic protons (i.e., cosmic rays and solar flares) in space. Such a reduction in travel time cannot be achieved using conventional rockets because of the lower exhaust velocities of the combustion gasses. The most developed propulsion concept is NTP, which is a very high temperature reactor. The problems of rapid startup and shutdown thermal transients must be addressed for an NTP rocket to use the hydrogen propellant most efficiently and prevent potential fuel failure. Researchers focused on the phenomena of rapid shutdown, previously not widely considered, when the reactor is shut down at the end of its required burn, and the fuel cools rapidly because of residual hydrogen in the flow channels and through blackbody radiation to space. Experiments on nuclear fuels have shown that overly rapid cooling causes hydrogen to collect along the grain boundaries and cause decohesion failure. This project sought to determine the maximum cooling rate and to balance the heat losses by convection and radiation with the decay heat of the fission products to prevent fuel failure.

Researchers also addressed a near-term problem with the supply of the heat-producing plutonium isotope plutonium-238 to power robotic missions on Mars and through the outer solar system. A limiting criterion on plutonium-238 production is the amount of plutonium-236 created. Because of the high gamma activity of one daughter product and the resulting occupational radiation exposure, plutonium-236 is limited to 2 parts per million. Research focused on optimizing the cooling times between chemical processing steps to reduce the plutonium-236 in the final product. The results of this research allow the use of plutonium containing higher amounts of plutonium-236 produced in test reactors, such as ATR, with applications for defense, environmental monitoring and space uses.



Serpent model for a nuclear thermal propulsion reactor showing various enrichment zones and control drums to maximum cooling rate and balance heat losses.

TALENT PIPELINE:

Students:

- Emory Colvin, Oregon State University
- Zane Emery, Cornell University
- Justina Freilich, Oregon State University
- Avery Grieve, University of Michigan
- Joseph Hafen, University of Idaho
- Joshua Rhodes, University of Tennessee at Knoxville
- Lorenzo Venneri, MIT
- Teyen Widdicombe, University of Idaho

PRESENTATIONS:

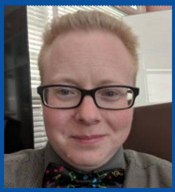
Cheu, D., J. Hafen, S. Herring, K. Judd, Q. Killian, A. Lesh, C. Nielsen, and A. Perry. 2020. "Modeling Chemical Reactions and Diffusion in an MMRTG Plutonium Pellet." Nuclear and Emerging Technologies for Space Conference. https://nets2020.ornl.gov/wp-content/uploads/2020/09/TRACK-1-Full-submission.pdf.

Colvin, E., B. Burt, L. Carpenter, S. Ercanbrack, J. Freilich, R. Herner, T.Kajihara, and J. Magnusson. 2020. "Optimization of Pu-238 production in the Advanced Test Reactor." Nuclear and Emerging Technologies for Space Conference. https://nets2020.ornl.gov/wp-content/uploads/2020/09/TRACK-1-Full-submission.pdf.

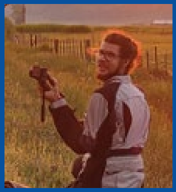
Kajihara, T., C. Godbole, and J. Magnusson. 2020. "Neutronic Analysis of the Submersion Subcritical Safe Space Reactor for Deploying LEU Fuel System Using Serpent." Nuclear and Emerging Technologies for Space Conference. https://nets2020.ornl.gov/wp-content/uploads/2020/09/TRACK-2-Full-submission.pdf.

Growing the Next Generation of Scientists and Engineers

The work on this LDRD project is contributing to three master's theses, authored by Emory Colvin, Joshua Rhodes, and Teyen Widdicombe.





Due to the COVID-19 pandemic, in 2020 the eight Center for Space Nuclear Research Summer Fellows participated virtually, from locations spread from New Hampshire to San Diego to Seattle. Top row left to right: Emory Colvin, Justina Freilich, Joe Hafen, Josh Rhodes, Lorenzo Venneri, Avery Grieve; Bottom row left to right: Teyen Widdicombe; Zane Emery.

A Hyphenated Separation Technique for Fuel Analysis Utilizing Gas Pressurized Extraction Chromatograph and Inductively Coupled Plasma – Quadrupole Mass Spectrometry

TOTAL APPROVED AMOUNT:
$542,000 over 2 years

PROJECT NUMBER:
19A39-099

PRINCIPAL INVESTIGATOR:
Matthew Jones, INL

CO-INVESTIGATORS:
Nick Erfurth, INL
Nicole Larson, INL
Cortney Pincock, INL
Brian Storms, INL

Researchers developed a novel liquid chromatography-mass spectrometry technique capable of providing real-time extraction chromatography data in a dropwise manner that can be quantitatively applied to nuclear fuel cycle samples for the determination of burn-up.

Quantitative analysis of nuclear fuel cycle samples is of the utmost importance for the validation of reactor modeling, qualification of nuclear fuel, post irradiation examination to understand fuel performance, and verification of burn-up credit for spent fuel storage and disposal. Lanthanides and actinides are among the most frequently requested analytes for these studies, but these analytes require chemical separations prior to quantification due to their overlapping signals. Following chemical separation, measurements must be made on a separate instrument which involves a great deal of sample handling and preparatory work. These additional efforts can be time intensive, costly, excessively wasteful, and prone to inaccuracy due to contamination risks and human error. The hyphenated liquid chromatography-mass spectrometry method developed in this project gives the analyst the ability to fine-tune the process to achieve the desired resolution and notice issues much sooner in the separation and measurement process, cutting down on wasted efforts that would otherwise be unavoidable in uncoupled systems. While there are liquid chromatography-mass spectrometry systems capable of taking these measurements in various ways, none of the chromatography systems previously coupled to mass spectrometers have the combination of high-resolution extraction chromatography microcolumns, small footprint, speed of separation, and relatively small volumes of waste that the gas pressurized extraction chromatograph boasts. Additionally, the researchers created a novel dropwise analysis method where each drop eluting from the gas pressurized extraction chromatograph column is collected and quantitatively analyzed utilizing the principle of isotope dilution mass spectrometry and a transient data analysis method known as least regression slope. This project exhibited an important advancement in separation technology given the growing applicability of extraction chromatography resins to the nuclear field and increased interest in small footprint microanalytical methods. The dropwise gas pressurized extraction chromatograph and inductively coupled plasma – quadrupole mass spectrometry system provides a simple cost-effective pathway to address any past, present, or undiscovered challenges that may occur during the development of the next generation nuclear fuel and reactor types.

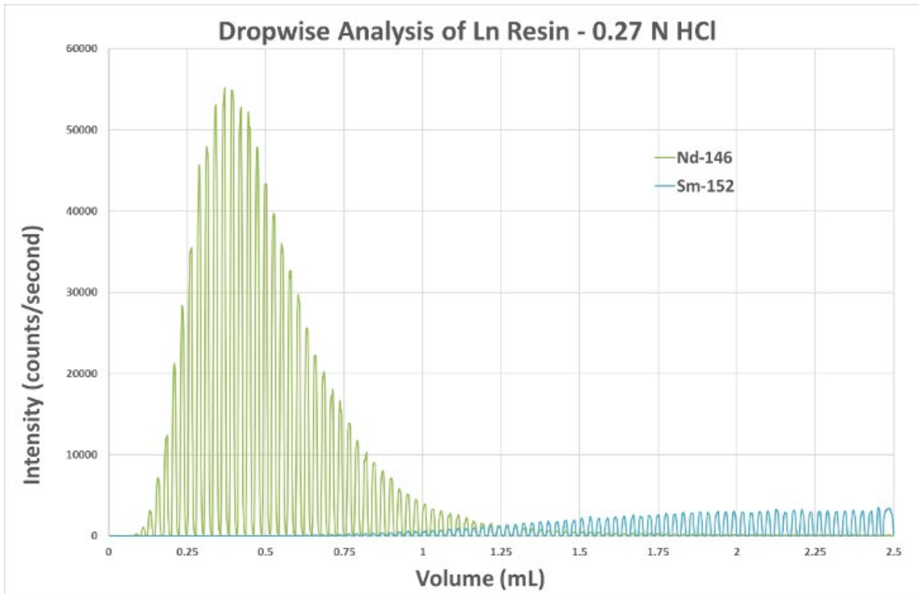
TALENT PIPELINE:

Student:

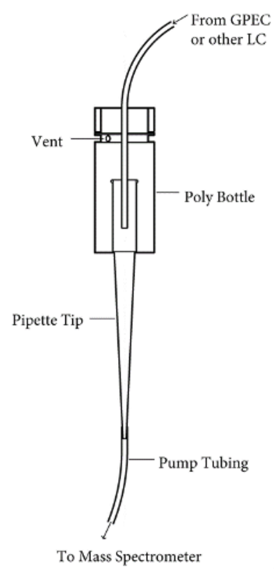
- Lashavio Little,
  Prairie View A&M

INTELLECTUAL PROPERTY:

One provisional patent application filed (BA-1150P): Dropwise Separation Analysis and Tandem Column Capabilities of Gas Pressurized Extraction Chromatography-mass Spectrometry



Example of raw data produced by the developed technique.



A diagram of the drop collector developed.

Coupling of Modeling and Experiment to Develop Predictive Models of the Mechanical Behavior of Nuclear Fuels and Materials

TOTAL APPROVED AMOUNT:
$926,800 over 3 years

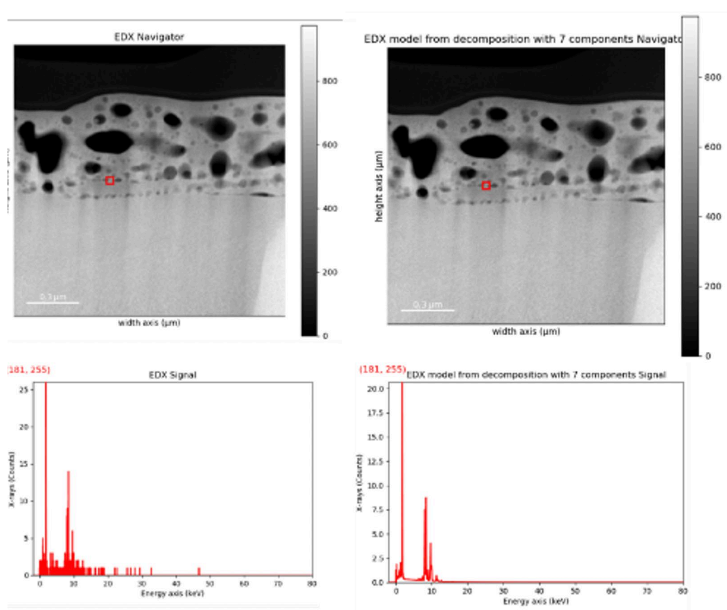
PROJECT NUMBER:
17P11-007

PRINCIPAL INVESTIGATOR:
Cheng Sun, INL
Russell L. Heath Distinguished Postdoctoral Researcher

CO-INVESTIGATORS:
Ge Yang, North Carolina State University
Yongfeng Zhang, INL

Researchers developed an innovative approach to correlating microstructure and mechanical properties at meso-scale and high-throughput data analysis methodologies using machine learning algorithms.

Predictive modeling and simulation have great potential to reduce the duration of the nuclear materials development cycle, which can take 10–20 years, but not enough focused experimental work has been done to develop and validate the models that will make this a reality. Demonstration of this potential requires the deliberate design of closely coupled modeling and experimental campaigns that generate results which can be compared on length scales consistent with model length scales. In this project, researchers developed an innovative approach to establish a correlation between microstructure and mechanical properties at meso-scale and high-throughput data analysis methodologies using machine learning algorithms. Suitable machine learning algorithms were applied to efficiently model energy dispersive X-ray spectroscopy datasets. Machine learning algorithms were also explored for feature extraction using the "complexity-minimizing" traits of reconstruction and implement high efficiency optimization algorithm to large scale X-ray spectroscopy datasets. This research demonstrated an innovative approach to measure the mechanical properties of materials at the meso-scale, the same with the modeling and simulation. The high-throughput mechanical testing shortens the development cycle of nuclear fuels and materials and thus expedite the discovery and design of advanced nuclear fuels and materials.



Singular value decomposition and principal component analysis for X-ray spectroscopy spectrum decomposition.

TALENT PIPELINE:

Students:

- Tanvi Ajantiwalay, University of Florida
- Xinchang Zhang, Missouri University of Science and Technology
- Panayotis Manganaris, University of Cincinnati
- Keyou Mao, Purdue University
- Myles Stapelberg, MIT

AWARDS:

- C. Sun, Early Career Exceptional Achievement Award, INL, 2019.
- K. Mao, Best Paper Award, Graduate Student Paper Contest, The Minerals, Metals, & Materials Society, 2019.

PUBLICATIONS:

Ajantiwalay, T., T. Trowbridge, A. Winston, C. Sun, K. Sridharan, and A. Aitkaliyeva. 2019. "Best Practices for Preparing Radioactive Specimens for EBSD Analysis." Micron, 118 (March):1-8. https://doi.org/10.1016/j.micron.2018.12.002.

Hany, I., G. Yang, C. E. Zhou, C. Sun, K. Gundogdu, D. Seyitliyev, E. O. Danilov, F. N. Castellano, D. Sun, and E. Vetter. 2019. "Low Temperature Cathodoluminescence Study of Fe-doped β-Ga2O3." Materials Letters, 257 (Dec.):126744. https://doi.org/10.1016/j.matlet.2019.126744.

Mao, K., C. Sun, Y. Huang, C. H. Shiau, et al. 2019. "Grain Orientation Dependence of Nanoindentation and Deformation-induced Martensitic Phase Transformation in Neutron Irradiated AISI 304L Stainless Steel." Materialia, 5 (March): 100208. https://doi.org/10.1016/j.mtla.2019.100208.

Mao, K., C. Sun, X. Liu, P. D. Freyer, F. A. Garner, H. J. Qu, and J. P. Wharry. 2020. "Effect of Laser Welding on Deformation Mechanisms in Austenitic Stainless Steel." Journal of Nuclear Materials, 528 (Jan.): 151878. https://doi.org/10.1016/j.jnucmat.2019.151878.

Mao, K., C. Sun, C. H. Shiau, K. H. Yano, et al. 2020. "Role of Cavities on Deformation-induced Martensitic Transformation Pathways in a Laser-welded, Neutron Irradiated Austenitic Stainless Steel." Scripta Materialia, 178 (March):1-6. https://doi.org/10.1016/j.scriptamat.2019.10.037.

PRESENTATIONS:

Sun, C. 2019. "Materials Research for Nuclear Energy Systems." Presented as a keynote speaker at the MIT Applied Energy A+B Symposium, (Cambridge, MA, May 22-24).

Mao, K. 2019. "Irradiation Assisted Deformation-induced Phase Transformation in Neutron Irradiated Austenitic 304L Stainless Steel Laser Weldment." Presented to the Minerals, Metals, & Materials Society 148th Annual Meeting & Exhibition (San Antonio, TX, March 10-14).

Growing the Next Generation of Scientists and Engineers

The work on this LDRD project formed the basis for one doctoral dissertation:

Mao, K. 2019. "Microstructural Characterization and Micromechanical Testing of Laser Weld Repairs on Neutron Irradiated 304 Stainless Steel." PhD diss. Purdue University.

From left to right, uranyl peroxide, uranium trioxide, and uranium dioxide produced through the uranium polishing process facilitated by LDRD research.

INTEGRATED FUEL CYCLE SOLUTIONS

Integrated fuel cycle solutions are necessary for sustaining and expanding nuclear energy in the future. Redefining the nuclear fuel cycle, with an emphasis on cost-effectiveness and waste minimization, is essential to addressing the needs of an aging fleet and developing the next generation of reactors to sustain and expand nuclear energy deployment. INL's integrated fuel cycle solutions S&T initiative supports the safe, secure, and economical management of nuclear fuel from inception to disposition.

Modeling and Simulation for Fuel Cycle Applications

INL's expertise and capabilities in nuclear chemical engineering are being applied to the modeling and simulation of elements of the nuclear fuel cycle separations. An LDRD project developed time-dependent and steady-state modeling tools for nuclear fuel cycle separation process design.[4]

These tools meet a critical need for advanced modeling and simulation capabilities to enable successful deployment of advanced nuclear fuel cycle technologies. The capabilities developed through this LDRD project have already been successfully applied in several subsequent R&D efforts, including high-assay low-enriched uranium (HALEU) polishing.

4 Project number 18A15-059: "Modeling and Simulation for Nuclear Fuel Cycle Separations Using Modular Coupling"

In Situ Investigation of Bond-structure and Local Chemistry in Molten Salts Using Optical and Electrochemical Techniques

TOTAL APPROVED AMOUNT:
$316,300 over 3 years

PROJECT NUMBER:
18P38-002

PRINCIPAL INVESTIGATOR:
Ruchi Gakhar, INL
Russell L. Heath Distinguished Postdoctoral Researcher

CO-INVESTIGATORS:
Qi An, University of Nevada, Reno
Dev Chidambaram, University of Nevada, Reno

Researches developed two unique capabilities applicable to the structural analyses of molten salt systems: the advanced spectroscopy furnace that can operate at temperatures up to 900°C, house multiple samples at the same time, and allows for combined *in situ* spectroelectrochemical measurements; and a computational approach for derivation of optical spectra of species at high temperatures.

The coordination chemistry of metals in various molten salt compositions has become an increasingly important area of research focused on both their formation mechanisms and their relationship with important processes such as electrolysis, corrosion, and other chemical processes relevant to the functionality of the molten salts for various industrial applications. Electronic absorption spectroscopy and electrochemistry are two powerful tools to investigate the molecular and electronic structure of the chemical species. However, their application to molten salts applications requires specialized tools and instrumentation considering the high radiation, elevated temperature, moisture sensitivity, and corrosive environments offered by the salts. This project designed the advanced spectroscopy furnace in response to this need to interrogate the chemical structure and speciation of molten salts using spectroscopy and electrochemical techniques simultaneously while maintaining the chemical integrity of molten salt samples. Several other spectroscopy techniques can also be coupled to the same furnace using additional ports. Combining experimental capabilities with a computational framework results in an effective high temperature electronic absorption spectroscopy technique for evaluation and fundamental understanding of molten salt chemistry. These novel capabilities advance scientists' ability to study the structural chemistry of molten salt in the nuclear fuel cycle and MSR technologies.

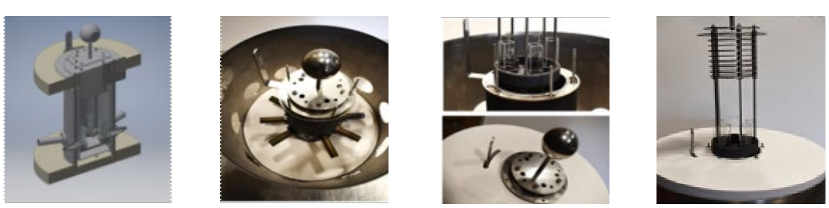
TALENT PIPELINE:

Students:

- Jon Fuller, University of Nevada, Reno
- William Phillips, University of Nevada, Reno

PUBLICATION:

Phillips, W., R. Gakhar, G. Horne, B. Layne, K. Iwamatsu, A. Ramos-Ballesteros, M. Shaltry, J. LaVerne, S. Pimblott, and J. Wishart. 2020. "Design and Performance of High-temperature Furnaces and Cell Holder for *in situ* Spectroscopic, Electrochemical, and Radiolytic Investigations of Molten Salts." Review of Scientific Instruments 91(8) (July): 083105. https://doi.org/10.1063/1.5140463.



Spectroelectrochemical furnace set up at INL's Energy Innovation Laboratory.

Generation and Radiolysis of Exotic Actinyl Oxidation States of Berkelium, Californium, and Einsteinium

TOTAL APPROVED AMOUNT:
$96,600 over 1 year

PROJECT NUMBER:
19A41-011

PRINCIPAL INVESTIGATOR:
Gregory Horne, INL
Russell L, Heath Distinguished Postdoctoral Researcher

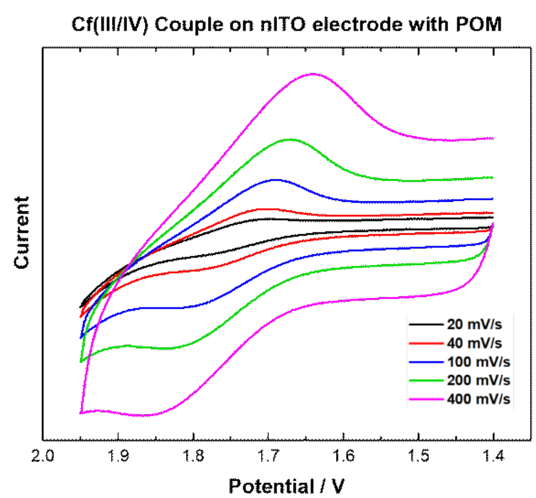
CO-INVESTIGATORS:
Travis S Grimes, INL
Tomas Albrecht-Schmitt, Florida State University
David Meeker, INL
Peter Zalupski, INL

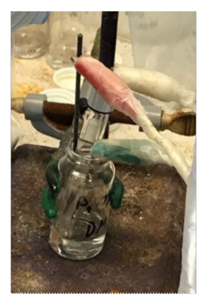
Leveraging a recent resurgence in higher oxidation state americium chemistry, researchers tested the novel concept that the remaining late actinides could be similarly manipulated to establish a new research area of late actinide high oxidation state chemistry.

The late actinides (americium onwards) are characterized not only by their relative scarcity, but also on the predominance of their trivalent oxidation state, limiting understanding of these exotic elements. Ionizing radiation and electrochemical techniques were employed to evaluate the feasibility of oxidizing the late trivalent actinides curium and californium in nitric acid solutions project scope was limited to curium and californium as berkelium and einsteinium became unavailable during the lifetime of this project. Despite a series of oxidation electrochemical experiments, californium(III) could not be oxidized to californium(IV) or higher but researchers did measure both oxidative and reductive radiation-induced reaction kinetics for aqueous curium(III) solutions. Similar reaction kinetics were also measured for curium(III). This novel research adds to our fundamental knowledge of the chemical properties of the late actinides, which is critical for the development of computer models that can be used to predict their behavior in a variety of nuclear fuel cycle scenarios.

TALENT PIPELINE:
Student:
- David Meeker, Florida State University

PRESENTATION:
Meeker, D. 2019. "Radiation-induced Redox Chemistry of 249Cf." Presented at the Miller Conference on Radiation Chemistry (Cumbria, UK, Sept.9-14).





Electrochemical oxidation of californium(III).

Radiation Chemical Kinetics of Actinide Redox Speciation

TOTAL APPROVED AMOUNT:
$389,300 over 3 years

PROJECT NUMBER:
18P38-001

PRINCIPAL INVESTIGATOR:
Gregory Horne, INL
Russell L. Heath Distinguished Postdoctoral Researcher

CO-INVESTIGATORS:
Thomas Albrecht-Schmitt, Florida State University
Andrew Cook, Brookhaven National Laboratory
Travis Grimes, INL
Stephen Mezyk, California State University, Long Beach
James Wishart, Brookhaven National Laboratory
Peter Zalupski, INL

Researchers established a unique capability for pico-second pulse radiolysis of radionuclides, defining the state of the art in the field of heavy element chemistry and providing critical insight into the chemical behavior of the actinide series.

Despite the importance of radiation-induced actinide redox speciation, fundamental understanding of their reaction mechanisms and associated kinetics is insufficient and necessitates a rigorous radiation chemistry research effort. This research aimed to understand the radiation-induced solution chemistry of the actinide series, and to ultimately predict their chemical behavior for a variety of chemical environments. Researchers performed an extensive suite of steady-state (external gamma and *in situ* alpha irradiations, via the self-radiolysis of actinide solutions) and ultrafast time-resolved pulsed electron irradiation measurements. These measurements were then coupled with quantitative, predictive, multi-scale computer modeling to provide a full theoretical description for radiolytic actinide redox speciation under envisioned conditions for advanced used nuclear fuel recycling scenarios. This work investigated uranium, americium, curium, and californium radiation chemistry. Results include a complete experimental and theoretical understanding for the radiation-induced redox chemistry of americium's penta- and hexavalent oxidation states; near completion of uranium irradiations electrochemical oxidation state manipulation, and predictive model compilation; and successful measurement of a series of americium/ligand reaction kinetics with the n-dodecane radical cation, highlighting at least an order of magnitude increase in ligand reactivity upon complexation. Concerning the latter, the ligands investigated included those of significant importance to the development of future used nuclear fuel reprocessing strategies. Consequently, this research advances the body of knowledge for recycling used nuclear fuel.

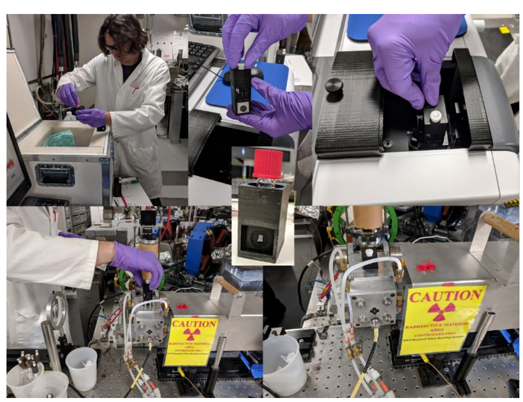
TALENT PIPELINE:

Student:

- David Meeker, Florida State University

PUBLICATION:

Horne, G., T. Grimes, W. Bauer, C. Dares, S. Pimblott, S. Mezyk, and B. Mincher. 2019. "Effect of Ionizing Radiation on the Redox Chemistry of Penta- and Hexavalent Americium." Inorganic Chemistry 5 8(13): 8551—855. https://doi.org/10.1021/acs.inorgchem.9b00854.



The capability to measure ultra-fast, radiation-induced actinide chemistry enables greater understanding of the solution chemistry of the actinide series.

Ortho-phosphoric and/or Phosphonic Acid Treatment of Aluminum-cladding and Aluminum-fuel Matrix (Fuel-meat) Spent Nuclear Fuel for Long-term Wet or Dry Storage Technique Development

TOTAL APPROVED AMOUNT:
$436,000 over 3 years

PROJECT NUMBER:
18P37-034

PRINCIPAL INVESTIGATOR:
Peter Zalupski, INL

CO-INVESTIGATOR:
Aleksey Rezvoi, Kairos Power

Researchers studied the galvanizing effect of phosphoric acid treatment to the corroded aluminum surfaces by applying a healing "safety shield" to aluminum surfaces to increase the safety of storage of spent aluminum-clad research reactor fuel.

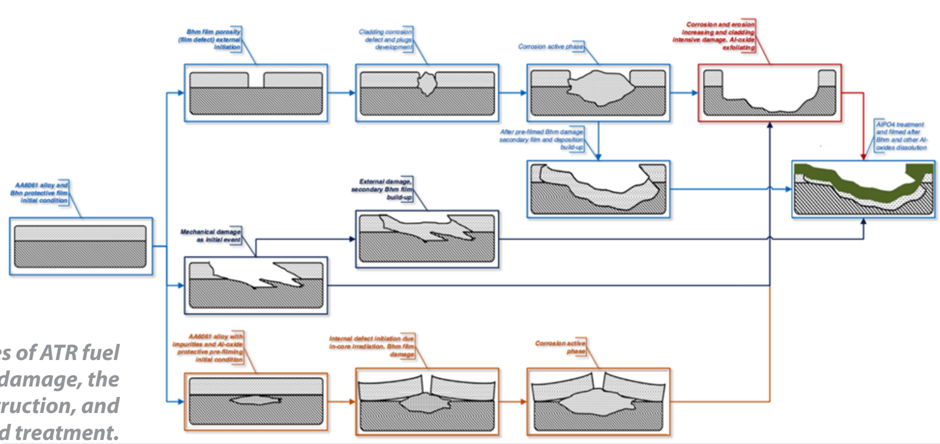
Research reactors widely use aluminum-clad nuclear fuel. In-reactor service and subsequent wet storage in cooling ponds exposes the aluminum surfaces to a combination of thermal, chemical, and radiolytic corrosion. As the corrosion penetrates the aluminum cladding, the concerns about the integrity of highly radioactive used fuel assemblies arise. DOE currently manages dry and wet storage of nearly 13 metric tons of aluminum-clad used nuclear fuel without a long-term storage solution. This research applied a galvanizing effect of phosphoric acid treatment to corroded aluminum surfaces to improve the stability of damaged aluminum-clad used nuclear fuel in preparation for long-term dry storage. Multiple chemical recipes were used, varying phosphoric acid concentration, equilibration time, temperature, and using additives such as nitric acid. In all experimental scenarios, the chemical passivation treatment yielded a complete removal of a top corrosion layer of bayerite, but boehmite proved very resilient to dissolution. Boehmite is a more compact oxyhydroxide corrosion layer on the aluminum surfaces, which is typically introduced on the surfaces of aluminum-clad nuclear fuel to enhance the corrosion robustness. The passivation layer of boehmite was very resilient to chemical treatment, pointing to an idea that another round of such treatment (after in-reactor service) could prolong the corrosion resistance of aluminum-clad used nuclear fuel and advance its long-term dry storage. The research outcomes for this project highlight the value of chemical pre-treatment of aluminum cladded nuclear fuel prior to reactor service.

TALENT PIPELINE:
Postdoc:

- Elizabeth Parker-Quaife, INL

INTELLECTUAL PROPERTY:
One IDR

PUBLICATION:
Parker-Quaife, E., C. Verst, C. R. Heathman, P. R. Zalupski, and G. P. Horne. 2020. "Radiation-Induced Molecular Hydrogen Gas Generation in the Presence of Aluminum Alloy 1100." Rad. Phys. Chem., 177: 109117. https://doi.org/10.1016/j.radphyschem.2020.109117.



Different types of ATR fuel element cladding damage, the advancement of destruction, and proposed treatment.

Modeling and Simulation for Nuclear Fuel Cycle Separations Using Modular Coupling

TOTAL APPROVED AMOUNT:
$676,600 over 3 years

PROJECT NUMBER:
18A12-059

PRINCIPAL INVESTIGATOR:
Kevin Lyon, INL

CO-INVESTIGATORS:
Valmor de Almeida, University of Massachusetts Lowell
Vivek Utgikar, University of Idaho

Researchers developed a modeling and simulation capability that can accurately predict liquid-liquid extraction process chemistry to aid in flowsheet design for a wide variety of hydrometallurgical separation technologies for the nuclear fuel cycle.

Hydrometallurgical separation processes have played a critical role in the nuclear fuel cycle since the inception of nuclear energy. Solvent extraction has been utilized at the industrial scale for the recovery of uranium from ore, uranium and plutonium recovery from irradiated nuclear fuel, and nuclear waste management. Despite widespread application in the nuclear fuel cycle, development of robust models that aid in the design, operation, and troubleshooting of advanced separation processes remains one of the most significant challenges in separation science. The need for advanced modeling and simulation capabilities is critical to enable successful deployment of advanced nuclear fuel cycle technologies. Furthermore, developing advanced separation technologies is a crucial step towards demonstrating proof of principle concepts for innovative actinide chemistry. This project developed time-dependent and steady-state modeling tools for nuclear fuel cycle separation process design. The modeling framework is a valuable capability for a vast array of other applications, such as safeguards and material protection, critical materials separations, and various mining and minerals hydrometallurgy applications. The capabilities developed under this project have been successfully used in several subsequent R&D efforts, including HALEU polishing.

Leveraging capabilities developed under this LDRD, INL researchers successfully removed chemical and radiological contaminants from HALEU, an essential feedstock for the development of next generation advanced thermal reactor fuels.

TALENT PIPELINE:

Students:

- Chaithanya Balumuru, University of Idaho
- Paige Brimley, University of Utah
- Clay Allred, University of Idaho
- Taha Azzaoui, University of Massachusetts Lowell
- Jarod Perko, University of Idaho

PRESENTATIONS:

Balumuru, C., V. Utgikar, and K. Lyon. 2020. "Hydrodynamics of Extraction Devices: Residence Time Distribution in Centrifugal Extractors for Organic Phase." Presented at the American Nuclear Society Winter Meeting, (Virtual Meeting, Nov. 16-19).

de Almeida, V., K. Lyon, and T. Azzaoui. 2018. "Design and Implementation of a Nuclear Solvent Extraction Plant-Level Simulator." Presented at the 18th AIChE Annual Meeting, Nuclear Engineering Division, (Pittsburgh, PA, Oct. 28-Nov. 2).

Lyon, K. 2019. "Solvent Extraction Flowsheet Modeling at INL: Approach, Current Interests, and Future Direction." Presented at the 3rd GENIORS Workshop, (Milano, IT, Nov. 4-6).

Growing the Next Generation of Scientists and Engineers

The work on this LDRD project formed the basis for one doctoral dissertation.

Lyon, K.L., 2020. "Advances in Solvent Extraction: Separation and Purification of Adjacent Trivalent Lanthanides Using the Electroneutral Solvating Extractant N,N,N',N'-Tetraoctyl Diglycolamide." Ph.D diss., University of Idaho.

Spectroscopic Studies of Covalency in Minor Actinide-soft Donor Ligand Complexes

TOTAL APPROVED AMOUNT:
$223,500 over 2 years

PROJECT NUMBER:
19P43-006

PRINCIPAL INVESTIGATOR:
Corey Pilgrim, INL
Glenn T. Seaborg Distinguished Postdoctoral Researcher

CO-INVESTIGATORS:
Christopher Colla, Lawrence Berkeley National Laboratory
Gauthier Deblonde, Lawrence Livermore National Laboratory (LLNL)
Harris Mason, LLNL
Mavrik Zavarin, LLNL

COLLABORATOR:
LLNL

This project studied the effects of covalency in the bonding environment between ligands and minor actinide species using nuclear magnetic resonance (NMR) spectroscopy. After crystallizing the complexes out of solution, the crystal structure was obtained and used as a starting point with density functional theory based computational methods to model the bonding environment.

Advanced nuclear fuel reprocessing schemes rely on the separation of the minor actinides from the lanthanides in highly ionic aqueous media. This separation is challenging, as the minor actinides and lanthanides are very similar in their chemistries with both sets of species forming similarly sized +3 cations in solution, with most of these ions also containing unpaired electrons (i.e., they become paramagnetic). The current model for separating these species relies on the exploitation of the differences in electronic structure, as the reactive electrons in the lanthanides reside within the 4f-orbitals while the reactive electrons in the minor actinides reside within the 5f-orbitals. NMR offered an alternative approach to study the effects and extent of the covalency differences between the complexes of minor actinides and lanthanides. NMR measures the chemical shift of nuclei within a static external magnetic field and can provide a fingerprint for molecules that is dependent on the connectivity and electronic structure of the molecule. Using NMR spectroscopy to explore the fundamental chemistry of actinides, creating synthetic schemes to crystallize the complexes from aqueous solution, and modeling the physical and electronic molecular structure advance nuclear fuel reprocessing capability.

Crystallization was achieved using a mixture of vapor-diffusion and slow-evaporation crystallization techniques with different aqueous/organic solvent mixtures. Crystals of the metal-ligand complexes slowly form diffraction-quality crystals for analysis.

Task-specific Ionic Compounds for In-field Sample Preparation

TOTAL APPROVED AMOUNT:
$385,700 over 2 years

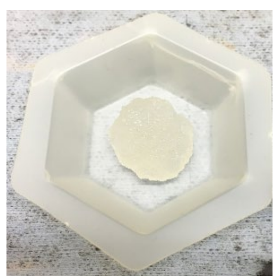
PROJECT NUMBER:
19A39-165

PRINCIPAL INVESTIGATOR:
Christopher Zarzana, INL

CO-INVESTIGATORS:
Rika Hagiwara, Kyoto University
Kumari Kavita Sharma, Idaho State University

Researchers synthesized a novel fluorinating ionic compound that is a solid at room temperature, which makes it a good candidate to be an operator safe, shipping compliant option for in-field sample dissolution.

In the event of a nuclear detonation, actinide and fission product-containing debris can be analyzed to provide information about the nature of the device. In-field sample dissolution prior to transport to a laboratory is critical for reducing the time between an event and delivery of information to decision makers. However, the best dissolution methods utilize liquid strong acid solutions, which are incompatible with field collection standard operating procedure. Solid materials are required that, when mixed with water in the field, can provide the strong digestion and dissolution properties of nitric and hydrofluoric acids. Fluorohydrogenate ionic liquids have shown a remarkable ability to dissolve a wide range of materials, from refractory actinide oxides to cementitious material such as calcium silicates. This project investigated the relationship between the structure of fluorinating ionic liquids and their physiochemical properties, in particular melting point, and their ability to dissolve refractory debris samples to gain the fundamental knowledge needed to design new fluorinating ionic compounds with melting points above 50°C and strong dissolution properties. A novel room-temperature solid fluorinating ionic compound was synthesized, and refractory material dissolution studies and physiochemical properties measurements are on-going. Results of this project support nuclear safety and nonproliferation goals.



A novel room-temperature fluorinating material.

Studies of Solubility and Reactivity of Fission Products (Cesium, Iodine, Tellurium, and Barium) in Primary Sodium

TOTAL APPROVED AMOUNT:
$190,000 over 2 years

PROJECT NUMBER:
19P43-004

PRINCIPAL INVESTIGATOR:
Yi Xie, formerly INL
Glenn T. Seaborg Distinguished Postdoctoral Researcher

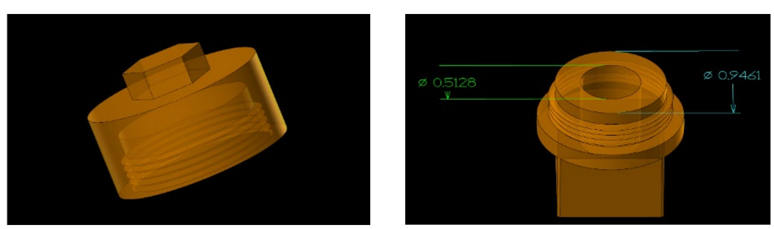
CO-INVESTIGATORS:
Michael Benson, INL
Jinsuo Zhang, Virginia Tech

Researchers developed a new experimental approach to investigate the solubility of fission products in molten sodium and the degradation effects of fission products on structural materials to better assess the safety of sodium-cooled fast reactors.

One concern in the use of nuclear energy is the potential release of radionuclides during normal and abnormal operations of reactors. With the redundant safety systems present in a sodium-cooled fast reactor, a radionuclide release is unlikely. To understand the consequences of a radionuclide release, the release itself needs to be investigated, as well as the final destination of the radionuclides, whether that is to remain in the sodium or to react and corrode the reactor structural materials. The safety assessment of sodium-cooled fast reactors requires a mechanistic-level understanding about the thermodynamics, chemistry, and corrosion of radionuclides in the fuel and coolant. The purpose of this project was to investigate the behavior of fission products in sodium to improve the understanding of the fission products retention capability of primary sodium in sodium-cooled fast reactors and the corrosion effects on structural materials. Researchers evaluated four typical fission products, based on the prevalence of the radionuclides in a sodium-cooled fast reactor, and addressed gaps in the current state of knowledge. A critical review of the solubility and corrosion in molten sodium was conducted. The corrosion effect on structural materials was studied by immersing the typical sodium-cooled fast reactor structural materials into molten sodium with tellurium. Microstructural analysis was conducted on the structural materials using scanning electron microscopy. This novel experimental setup to test materials' corrosion in molten sodium advances the ability to assess reactor fuel safety and to develop structural materials.

TALENT PIPELINE:
Students:

- Weiqian Zhuo, Virginia Tech
- Jimmy Burke, Virginia Tech



Customized crucibles, made of titanium alloy, with a threaded lid, were designed and fabricated for the test to prevent the vaporized sodium from leaking.

Solvent Radiolysis Product Production Using Preparative High-performance Liquid Chromatography

TOTAL APPROVED AMOUNT:
$366,500 over 3 years

PROJECT NUMBER:
18A12-082

PRINCIPAL INVESTIGATOR:
Christopher Zarzana, INL

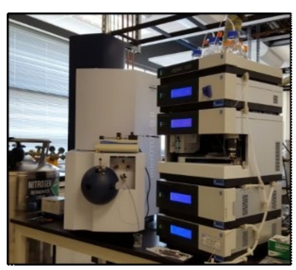
CO-INVESTIGATOR:
Kumari Kavita Sharma, Idaho State University

Researchers developed cost-efficient methods for producing standards of the radiolytic degradation products of ligands that aid separating used nuclear fuel.

Solvent systems used for spent nuclear fuel separation are subject to intense radiation fields from the spent fuel, resulting in a degradation of separation performance over time from both the radiolytic destruction of active compounds and the production of degradation compounds. Development of a quantitative understanding of the effects of radiolysis on separations is impeded by a near-complete lack of availability of degradation products from chemical manufacturers. Synthesis of these degradation products through traditional means is both cost and time prohibitive, inhibiting advancement of new fuel separation processes. As an alternative, a semi-preparative high-performance liquid chromatography method was developed to purify the radiolytic degradation products of tetraoctyldiglycolamide, a ligand designed to separate lanthanides and actinides from dissolved used nuclear fuel. Researchers first prepared degradation products by irradiating high concentrations of ligand to high doses before separating and purifying degradation products using preparative-scale high-performance liquid chromatography. The final step was to evaporate high-performance liquid chromatography mobile phase from the collected products with a vacuum concentrator. Using this new method, small quantities of tetraoctyldiglycolamide degradation products were produced for use as mass spectrometry standards and a higher through-put method is currently being evaluated. Using this new method to separate molecule degradation products at minimal cost enables the fundamental research that will accelerate the development of advanced, integrated fuel cycles.

TALENT PIPELINE:
Students:

- James Kirkby, Carnegie Mellon University
- Kyle Riggs, University of Idaho
- Samuel Tyndall, Miami University, Ohio
- William Yik, Harvey Mudd College
- Wells Crosby, Century High School



Researchers prepared degradation products by irradiating high concentrations of ligand to high doses, then separated and purified degradation products using preparative-scale high-performance liquid chromatography, and then evaporated high-performance liquid chromatography mobile phase with a vacuum concentrator.

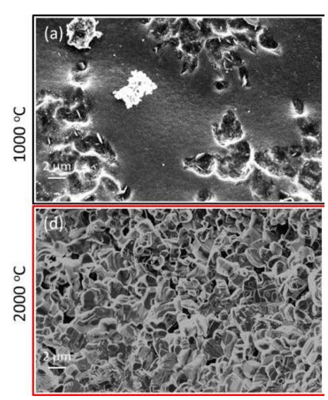
INL's Dynamic Energy Transport and Integration Laboratory supports RD&D efforts to ensure that future energy systems will be flexible and responsive.

INTEGRATED ENERGY SYSTEMS

Innovative technologies and advances in energy-generation sources, storage, and delivery are needed to reduce environmental impact via reduced emissions across all energy sectors, reduced water use, and production of clean-water resources while maintaining economic competitiveness. INL researches and demonstrates methods to harness and use a variety of forms of nuclear energy products (radiation, heat, and electrons) in conjunction with energy products from other clean-energy sources to accelerate the deployment of an economy based on clean, reliable, and sustainable energy. INL's integrated energy systems S&T initiative works to pave the way for eventual systems adoption by commercial producers and consumers through at-scale demonstration of integration of diverse energy generation sources and technologies to harness heat and electricity from generation for industrial process, such as hydrogen production.

Discovery Could Help Fine-tune Carbon Microstructure

Coal and diamonds are both composed of carbon, but the two materials differ in their microscopic arrangement of atoms, or microstructure, leading to differences in appearance, conductivity, hardness, and other properties. Optimizing carbon microstructure could benefit applications in energy storage, sensors, and next generation nuclear material systems. A group of INL researchers used LDRD funds to identify how the final microstructure varied depending on the temperature and the starting material. The work aimed to provide a road map with short-cuts to speed up the search for appropriate heat treatments to create carbon composite materials with the desired microstructure, which varies by application. In addition to experimental work, the INL group also did simulations that modeled how the fibers and films would evolve during heat treatment. The group's findings could lead to industry adoption of improved precursors and processes to yield preferred nano-structures for specific applications.



Carbon thin films arrange differently depending on the treatment temperature.

Effect of Strong-coupled Defects, Structure, Compositions, and Morphology of Advanced Energy Materials on Electrochemical Performance: A Case Study of Co-production of Ethylene and Specialty Chemicals Using Ethane and Carbon Dioxide at Intermediate Temperatures

TOTAL APPROVED AMOUNT:
$728,100 over 2 years

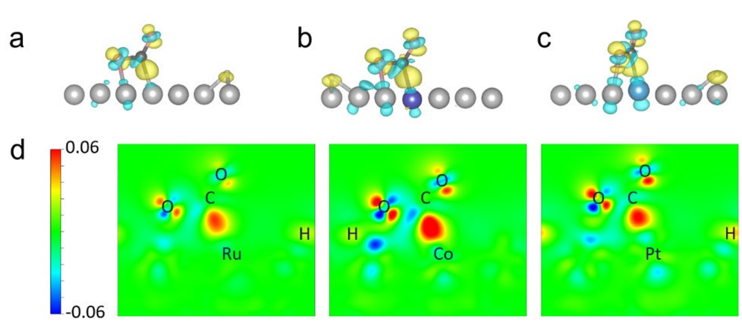
PROJECT NUMBER:
19A39-096

PRINCIPAL INVESTIGATOR:
Dong Ding, INL

CO-INVESTIGATORS:
Yipeng Gao, INL
Lucun Wang, INL
Jianguo Yu, INL

Researchers successfully developed a novel multiscale computational framework to guide development of advanced electrochemical membrane reactors, with a special emphasis on the case of co-production of ethylene and chemicals using ethane and carbon dioxide as the feedstocks at intermediate temperatures.

For the integrated energy systems of the future to operate economically and efficiently, it is necessary to develop systems that leverage the heat and electricity from nuclear energy and renewables as energy inputs in an electrochemical system. One such system could co-produce ethylene and chemicals using ethane and carbon dioxide. Rather than relying on potentially expensive and time-consuming trial and error, a computational framework addressing the challenges of the integrated systems could speed development and deployment. Researchers established a novel multiscale framework of developing advanced energy materials for electrochemical manufacturing. The framework provides insight for rational design of materials, interfaces, and morphology by addressing the basic science needs for this specific application, greatly reforming the time-consuming trial-and-error experimental efforts. The framework has been demonstrated to be effective for rational design of active and robust catalysts towards carbon dioxide protonation reaction by density functional theory calculations. In conjunction with phase field modeling in optimizing the electrode microstructure for fast mass/charge transport kinetics, the superior electrochemical performance is confirmed by rational design of several new electrocatalysts and novel electrode microstructure. New catalysis and electrocatalysis evaluation facilities have been established with fully equipped capabilities of high temperature carbon dioxide hydrogenation and protonation tests. These facilities allow for quick screening of the prepared catalysts that can be incorporated into the electrochemical cells for further tests, enabling efficient material/catalyst R&D. This framework supports leveraging the heat and electricity from the nuclear energy and renewables as energy inputs in an electrochemical system.



Enhanced interaction of adsorbed carbon dioxidemolecules and the catalyst surface has been validated. (a-c) The calculated charge density difference between the catalyst surface and adsorbed carbon dioxide and hydrogen intermediates. Yellow and cyan isosurfaces exhibit the accumulation and depletion of electron densities at the isovalue of 0.006 $e^-/Bohr^3$. (b) The 2D projection of electron density difference at the surfaces clearly maps out the higher electron accumulation between carbon and cobalt or platinum than that between carbon and ruthenium.

TALENT PIPELINE:

Postdocs:

- Bin Hua, INL
- Meng Li, INL

Student:

- Clarita Regalado Vera, New Mexico State University

INTELLECTUAL PROPERTY:

One U.S. provisional patent application filed (62/706,510): Catalysts with Tunable Electrocatalytic Behavior for Efficient CO2 Electrochemical Conversion at Intermediate Temperatures

Two IDRs

PUBLICATIONS:

Ding, H., W. Wu, and D. Ding. 2019. "Advancement of Proton-Conducting Solid Oxide Fuel Cells and Solid Oxide Electrolysis Cells at Idaho National Laboratory (INL)." ECS Transactions. 91(1): 1029-1034. https://doi.org/10.1149/09101.1029ecst.

Gao, S., R. Wang, C. Ma, Z. Chen, Y. Wang, M. Wu, Z. Tang, N. Bao, D. Ding, W. Wu, F. Fan, and W. Wu. 2019. "Wearable High-dielectric-constant Polymer with Core-shell Liquid Metal Inclusions for Biomechanical Energy Harvesting and Self-powered User Interface." Journal of Materials Chemistry A. 7(12): 7109-7117. https://doi.org//10.1039/C9TA01249D.

Tang, W., J. Jian, G. Chen, W. Bian, J, Yu, H. Wang, M. Zhou, D. Ding, and H. Luo. 2020. "Carbon-nanotube Supported MoS_2 via Microwave-Heating for Enhanced Performance of Hydrogen Evolution." Energy Materials Advances 2021:8140964. https://doi.org/10.34133/2021/8140964.

Ye, R.-P., L. Lin, L.-C Wang, D. Ding, Z. Zhou, P. Pan, Z. Xu, J. Liu, H. Adidharma, M. Radosz, and M. Fan. 2020. "Perspectives on the Active Sites and Catalyst Design for the Hydrogenation of Dimethyl Oxalate." ACS Catalysis 10(8): 4465-4490. https://doi.org/10.1021/acscatal.9b05477.

Wang, H., X. Chen, D. Huang, M. Zhou, D. Ding, and H. Luo. "Cation Deficiency Tuning of $LaCoO_3$ Perovskite as Bifunctional Oxygen Electrocatalysts." ChemCatChem 12 (10): 2768-2775. https://doi.org/10.1002/cctc.201902392.

Wang, H., L. Yan, T. Nakotte, W. Xu, M. Zhou, D. Ding, and H. Luo. 2019. 2019. "IrO_2-incorporated $La_{0.8}Sr_{0.2}MnO_3$ as Bifunctional Oxygen Electrocatalysts with Enhanced Activities." Inorganic Chemistry Frontiers 6(4): 1029-1039. https://doi.org/10.1039/C9QI00033J.

Wang, L.-C., Y. Zhang, J. Xu, W. Diao, S. Karakalos, B. Liu, X. Song, W. Wu, T. He, and D. Ding. 2019. "Non-oxidative Dehydrogenation of Ethane to Ethylene over ZSM-5 Zeolite Supported Iron Catalysts." Applied Catalysis B: Environmental 256: 117816. https://doi.org/10.1016/j.apcatb.2019.117816.

Xu, W., N. Apodaca, D. Ding, L. Yan, G. Chen, M. Zhou, P. Choudhury, and H. Luo. 2019. "A-site Excessive $(La_{0.8}Sr_{0.2})_{1.05}MnO_3$ and $(La_{0.8}Sr_{0.2})_{1.1}MnO_3$ Perovskite Oxides for Bifunctional Oxygen Catalyst in Alkaline Media." ACS Catalysis 9(6): 5074-5083. https://doi.org/10.1021/acscatal.9b00800.

Carbon: Interfaces, Structure, and the Impacts on Performance

TOTAL APPROVED AMOUNT:
$1,136,600 over 2 years

PROJECT NUMBER:
19A39-139

PRINCIPAL INVESTIGATOR:
Eric Dufek, INL

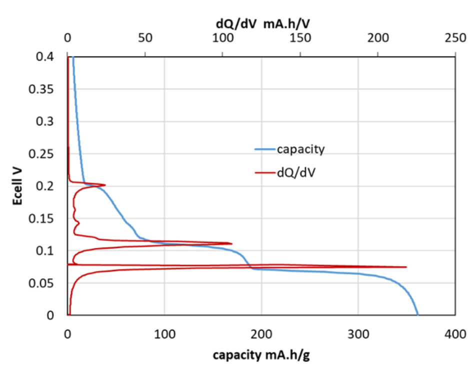
CO-INVESTIGATORS:
Rebecca Fushimi, INL
Josh Kane, INL
Lan Li, Boise State University
Zachary Thompson, INL
Will Windes, INL
Hui Xiong, Boise State University

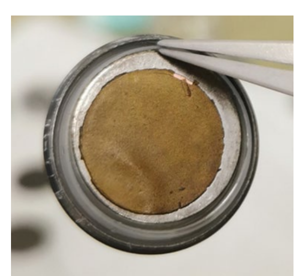
Researchers made several key advancements in both the theoretical and experimental activities which provide key insight into how carbon allotropes behave across different environments including lithium diffusion in graphite with defects, the evolution and migration of surface oxygen species, and the electrochemical variation in carbon surfaces.

Carbon plays a significant role in many energy related fields including nuclear graphite, high temperature structural components, batteries, catalysis, and advanced sensor and filter technologies. Scientists enhanced understanding across length scales and to better quantify variation between atomic level heterogeneity and defects with bulk characteristics. Researchers sought to understand surface evolution during oxidation, surface energy variations due to defects, and the inherent reactivity of graphite at different stages of lithiation. One of the primary challenges of establishing the core structure-property-reactivity relationships within carbon is the nearly infinite variability in the carbon chemical and microstructure, which can affect the chemical and electrochemical reactivity. However, at relevant length scales for energy applications, a plethora of defects exist. These defects within and between the basal planes locally modify electronic bond potential and thus chemical reactivity of the carbon surface. To gain a greater understanding of these defects, researchers combined computational, electrochemical, physical, and temporal analysis to derive structure-function relationships and created distinct samples using both commercial and modified sources including electrochemical and thermal modification. This combination of theoretical and experimental activities resulted in insights in transport/surface diffusion of samples during oxidation and how lithium moves through graphitic structures with varying degrees and types of defects. The results of this project target developing new means to prepare carbon allotropes for energy applications.

TALENT PIPELINE:
Postdocs:
- Rakesh Batchu, INL
- Zongtang Fang, INL
- Ningshengjie Gao, INL
- Yuxiao Lin, INL
- Haoyu Zhu, Boise State University

Electrochemically lithiated graphite stages and image of lithiated graphite electrode used for temporal analysis of products experiments.





A Longitudinal Finned Heat Exchanger for Subsurface Thermal Storage and Recovery

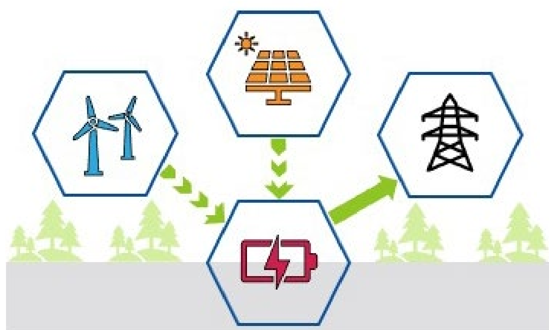
TOTAL APPROVED AMOUNT:
$10,000 over less than 1 year

PROJECT NUMBER:
20A1047-034

PRINCIPAL INVESTIGATOR:
Robert Podgorney, INL

Development of a longitudinal finned heat exchanger for storing and recovering heat in porous and crystalline rocks using only a single well in a countercurrent heat exchange design has the potential to significantly advance subsurface thermal energy storage.

Subsurface thermal energy storage is a concept where geologic formations can be used as a battery, storing thermal energy collected during periods of excess generation or availability, making it available at later times. Previous studies performed viability evaluations utilizing conventional well configurations to store heat within subsurface porous media (e.g., oil reservoirs) with optimistic results. In operation of the proposed novel longitudinal finned heat exchanger, fluid would be gravity fed into the large diameter boring, where it could enter the heat exchange fins, and travel downward to be later extracted near the bottom of the smaller diameter boring and pumped to the earth's surface to be used for several beneficial purposes, namely generating baseload electricity or process heat. The heat exchange fins would only be open to the well bores at the top and bottom. The technology proposed allows for either heated or ambient temperature fluids to be injected, allowing thermal energy storage in the subsurface. This LDRD project ended early when outside funding was secured.



Viable subsurface energy storage solutions may enable intermittent renewables, such as wind and solar, to transition to baseload power generation.

Investigation of Exciton Delocalization and Exciton Coherence in Chromophores and Acoustic Nanostructures

TOTAL APPROVED AMOUNT:
$1,147,700 over 3 years

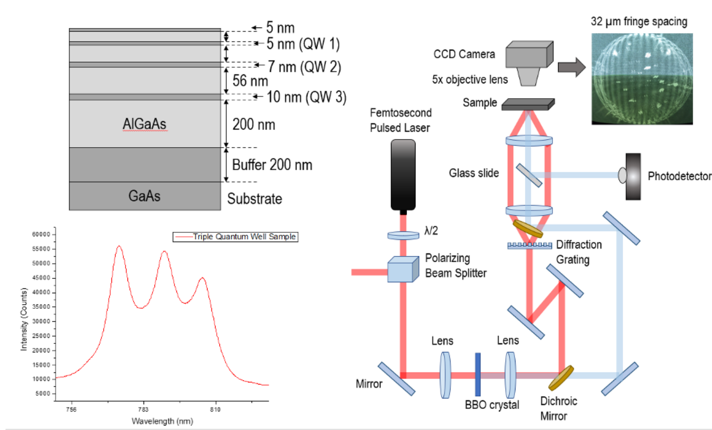
PROJECT NUMBER:
17P11-030

PRINCIPAL INVESTIGATOR:
David Hurley, INL

CO-INVESTIGATORS:
Bill Knowlton, Boise State University
Ryan Pensack, Boise State University
Robert Schley, INL
Paul Simmonds, Boise State University
Bernard Yurke, Boise State University

To advance the feasibility of room-temperature quantum materials systems, researchers developed the foundation for configuring and testing excitonic devices in molecular systems and solid-state systems, two complementary systems for the realization of universal quantum computers and other applications.

Quantum materials have a rich potential for providing transformative energy technologies ranging from new energy efficient computation paradigms to lossless energy transport across the national grid. The field of quantum materials, however, is still in its infancy with many quantum materials systems requiring cryogenic temperatures to be viable. With this project, researchers accomplished two main goals in advancing room-temperature quantum materials systems: first, advance the science for demonstrating room temperature exciton delocalization in two excitonic systems; and second, build capacity and expertise in developing and understanding quantum materials. Researchers first identified various chromophore types, number of chromophores, and nucleic acid scaffolds that will form aggregates with superior coherent excitonic delocalization before designing, construction and testing a system for acoustic phonon confinement of excitons in a prototypical solid-state system. The project then focused on demonstrating exciton delocalization and coherence of Frenkel and Wannier-Mott excitons before building a theoretical framework that describes the optical signatures of Frenkel excitons in chromophore aggregates and behavior of Wannier-Mott excitons in solid-state systems. This work demonstrated exciton delocalization in Wannier-Mott systems and developed experimental capability need to confine and measure exciton localization using high frequency, laser generated surface acoustic phonons. By advancing understandings of room-temperature quantum materials systems, this fundamental materials science project advanced new paradigms for realizing quantum computation systems.



Quantum confinement using the acousto-electric field associated surface acoustic phonons. Upper left: Quantum well geometry. Bottom left: Photoluminescence spectra of three buried quantum wells. Right: Design of new method that employs transient absorption gratings defined by interfering two laser beams.

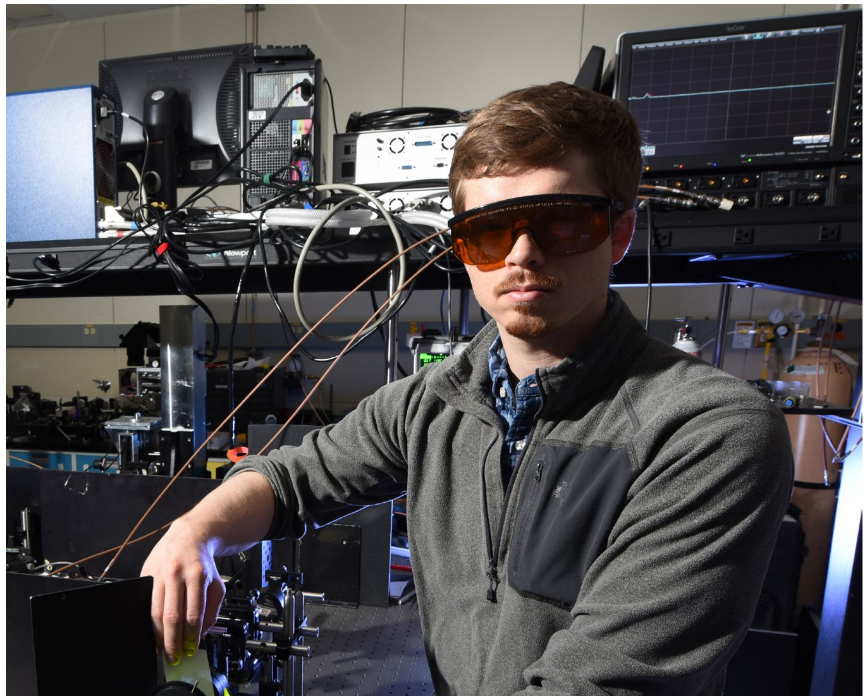
TALENT PIPELINE:

Postdocs:

- Cody Dennett, INL
  Russell L. Heath Distinguished Postdoctoral Researcher
- Amey Khanolkar, INL
  Russell L. Heath Distinguished Postdoctoral Researcher

Students:

- Allison Christy, Boise State University
- Jonathan Huff, Boise State University
- Lance Patton, Boise State University
- Simon Roy, Boise State University
- Kevin Vallejo, Boise State University
- Taylor Farmer, Boise State university



Cody Dennett earned his doctorate in nuclear science and engineering from MIT. He came to INL as a Distinguished Postdoctoral Researcher to leverage the Laboratory's unique capabilities in in situ material property characterization to explore degradation and evolution phenomenon. Dennett's work advances innovation in materials for harsh and extreme conditions.

PUBLICATION:

Huff, J.S., P.H. Davis, A. Christy, D.L. Kellis, N. Kandadai, Z.S.D. Toa, G.D. Scholes, B. Yurke, W.B. Knowlton, and R.D. Pensack. 2019. "DNA-templated Aggregates of Strongly-coupled Cyanine Dyes: Nonradiative Decay Governs Exciton Lifetimes." Journal of Physical Chemistry Letters 10:2386–2392. https://doi.org/10.1021/acs.jpclett.9b00404.

PRESENTATION:

Yurke, B. 2019 "Exciton quantum walks over DNA-assembled dye aggregates – A path to quantum computing?" Invited presentation at the Foundations of Nanoscience (FNANO) Conference (Snowbird, UT, April 15–18).

Investigation of Power Electronics and Control Systems for Nuclear/ Renewable Energy Parks

TOTAL APPROVED AMOUNT:
$125,000 over 1 year

PROJECT NUMBER:
20A1049-027

PRINCIPAL INVESTIGATOR:
Yusheng Luo, INL

CO-INVESTIGATORS:
SM Shafiul Alam, INL
Michael Heben, University of Toledo
Ning Kang, INL
Raghav Khanna, University of Toledo
Tyler Westover, INL

INL scientists advanced the feasibility of future integrated energy systems by developing an interface that allows nuclear power plants to rapidly dispatch electricity to both industrial users and the power grid while maintaining grid stabilization and resiliency.

Light-water nuclear reactors are in economic competition with natural gas combined-cycle power plants and wind and solar power generation in areas where these alternative energy options can drive the marginal cost of electricity below the baseload cost of carbon-free nuclear generation. Economics require that nuclear power plants develop non-electric markets as well as means to rapidly switch power between different customers. Researchers developed a novel high level interface controller for integrated energy systems that includes nuclear generation, hydrogen production, renewable generation, and dispatchable power consumption to enable nuclear power plants to rapidly dispatch electricity among closely connected industrial users and the bulk electric grid. Importantly, this control interface was automated to respond to power imbalances in less than 0.1 seconds, which is necessary to maintain frequency stability on the power grid. Researchers developed a novel approach to integrated energy systems by combining a rapidly dispatchable power load (hydrogen production) to steady nuclear generation, intermittent photovoltaic power generation, battery energy storage systems, and buildings that are also configured to actively dispatch power consumption. Modularized control systems contribute to the viability of efficiently and economically integrating nuclear power plant and hydrogen plants to enable the production of non-electrical products using nuclear power.

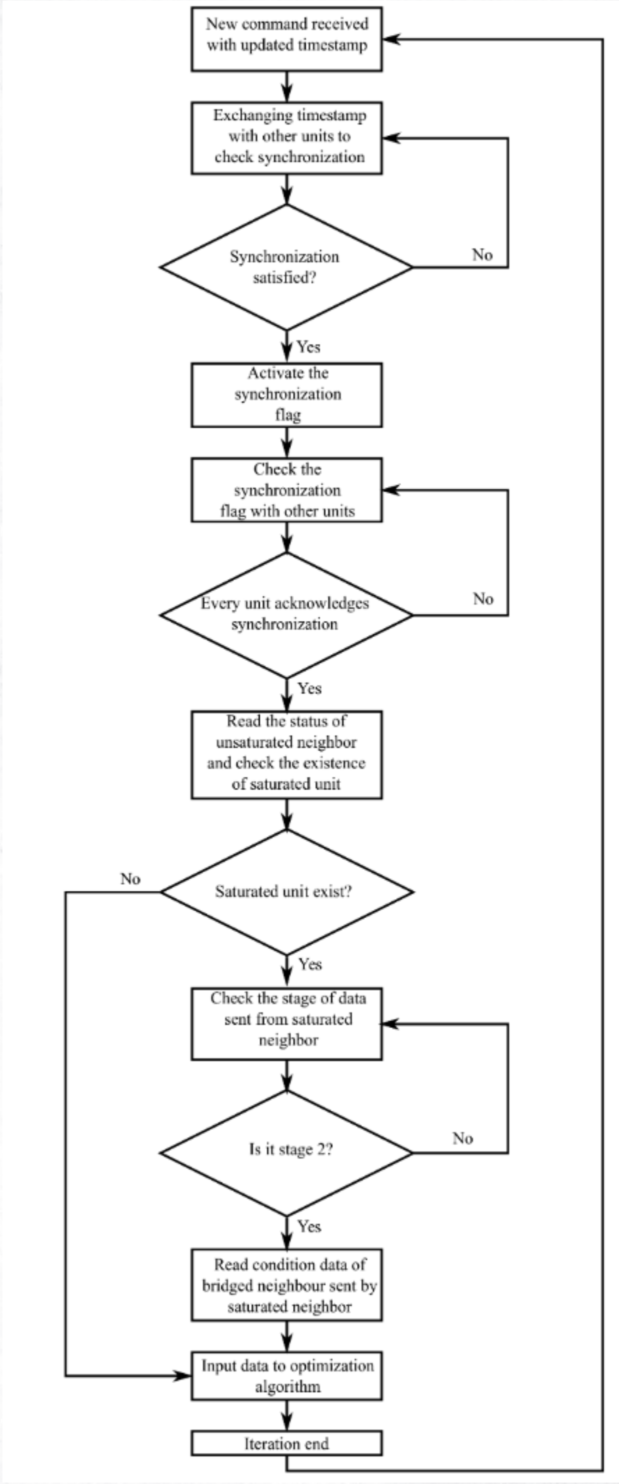
TALENT PIPELINE:

Student:

- Dave Raker, University of Toledo

PUBLICATION:

Luo, Y., C. Chen, R. Kadavil, B. Liaw, E. Muljadi, W. Wu, S.K. Srivastava, T. Mosier, and E. Dufek. 2020 "A Novel Framework for Optimizing Ramping Capability of Hybrid Energy Storage Systems." IEEE Transactions on Smart Grid. https://doi.org/10.1109/TSG.2020.3023712.



An example of the logic flow of software module developed for integrating rapid optimization algorithm in real-time operation environment.

Enabling Highly Scalable Multiphysics Simulation of Particulate Systems on Exascale Computing Architectures

TOTAL APPROVED AMOUNT:
$913,800 over 3 years

PROJECT NUMBER:
18A12-080

PRINCIPAL INVESTIGATOR:
Yidong Xia, INL

CO-INVESTIGATORS:
Laxmikant Kale, University of Illinois at Urbana-Champaign
Joshua Kane, INL
Zhen Li, Clemson University
Hong Luo, North Carolina State University
Lixiang Luo, ORNL
Yu-Hang Tang, Lawrence Berkeley National Laboratory
Tyler Westover, INL
Aaron Wilson, INL

Multiple state-of-the-art, high-performance computing (HPC)-enabled particle multiphysics simulation packages were developed for particle flow and mechanics modeling particularly applicable to the flow of fluids in shale.

The development of particle flow and mechanics modeling technologies that can scale to HPC for non-homogeneous mesoscale systems (e.g., flow of hydrocarbon and fracturing of source rocks) is a previously unexplored research area. Particle flow and mechanics simulations in those systems exhibit high spatial and temporal variabilities. Traditional parallel strategies can lead to severe load imbalance across processors and poor parallel efficiency (< 10%) on HPC, making it impossible to reach the required physical scales. To enable scalable HPC simulations for non-homogeneous particle flow and mechanics, researchers developed state-of-the-art HPC simulation toolkits including: a portable parallel computational framework, HTM3D, for enabling the R&D of particle-mesh coupled multiphysics simulators; an open-source particle simulator, userMESO 2.5, for fluid flow in mesoporous (nano- to micro) geomaterials; and two open-source image processing and analysis packages, IMG2VOX and VOX2DPD, for creating pore network voxels from 3D image stack (e.g., of geomaterials and nuclear materials) and converting voxels to standard particle data for simulation setup. These tools solve the problem of HPC scalability for particle flow and mechanics modeling and apply broadly to geothermal technologies, thermal-hydraulics in micro-reactors, and powder-based advanced manufacturing applications.

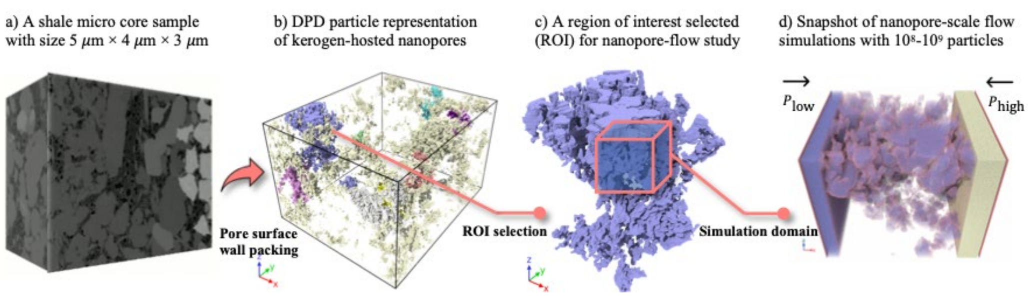


Illustration of a production-level shale analysis workflow from nanometer-resolution digital rock imaging to graphics processing unit (GPU)-accelerated many-body dissipative particle dynamics (DPD) simulations of fluid flow in realistic nanopores in shale.

TALENT PIPELINE:

Postdocs:

- Jiaoyan Li, INL
- Qi Rao, INL

Students:

- Ansel Blumers, Brown University
- Jan Goral, University of Utah
- Sam White, University of Illinois at Urbana-Champaign

AWARD:

- Best Research Poster Award at SC19, the world's largest annual HPC conference.

PUBLICATION:

Xia, Y., A. Blumers, Z. Li, L. Luo, Y.-H. Tang, J. Kane, H. Huang, M. Andrew, M. Deo, and J. Goral. 2020. "A GPU-accelerated Package for Simulation of Flow in Nanoporous Source Rocks with Many-body Dissipative Particle Dynamics." Computer Physics Communications 247: 106874. https://doi.org/10.1016/j.cpc.2019.106874.

PRESENTATION:

Xia, Y., L. Luo, A. Blumers, J. Kane, J. Goral, Y.H. Tang, Z. Li, H. Huang, and M. Deo. 2019. "Nanoporous Flow Simulations on the Summit Supercomputer." Poster presented at The International Conference for High Performance Computing, Networking, Storage, and Analysis (Denver, CO, Nov. 17-20). https://sc19.supercomputing.org/proceedings/tech_poster/tech_poster_pages/rpost108.html

INL's Sawtooth supercomputer became available to researchers in early 2020. Sawtooth ranks #37 on the 2019 list of the Top 500 and has the computing power to run complex modeling and simulation applications.

The world's largest SPS system, a Direct Current Sintering-800, is installed at INL providing a new unique capability that will leverage LDRD discoveries to push the boundaries of powder metallurgical processing techniques.

ADVANCED DESIGN AND MANUFACTURING FOR EXTREME ENVIRONMENTS

INL focuses on advanced materials and manufacturing solutions for use in extreme environments, including advanced nuclear reactors, defense systems, and space applications. INL, often in partnership with industry, seeks to discover and advance materials that must function in extreme environments for instrumentation and energy technologies. Addressing the nexus of material development, component fabrication, and qualification, from feedstock material through product validation will increase the performance and economic competitiveness of materials used in extreme environments. INL's advanced design and manufacturing for extreme environments S&T initiative accelerates discoveries and advances in materials for extreme environments, instrumentation, and energy technologies through adaptation, analysis, development, and integration of new or novel techniques.

Intensifying Advanced Manufacturing Processes

Through LDRD, INL answers basic science questions around new types of materials manufacturing technologies and explores materials developed through these manufacturing processes. The spark plasma sintering (SPS) manufacturing processes, an additive manufacturing process that uses electrical current to assist the sintering process and allows the manufacturing of materials at lower temperature, nearly 1000s degrees lower, and pressures than traditional manufacturing processes may have multiple applications for materials fabrication for extreme environments. Several recent LDRD projects serve as foundational research as INL grows its understanding of the possibilities of the SPS advanced manufacturing process. Project outcomes include: building a comprehensive model of process and materials microstructure evolution from individual powder particles to meter scale parts under the influence of electric fields, currents, temperature, and pressure simultaneously; developing a micro-SPS unit that enables *in situ* X-ray observation and characterization of SPS processing at length scales from micron to millimeter; and designing and fabricating a nano-SPS unit to achieve a 3 orders of magnitude decrease in observable length scales during SPS processing.

Rapid Design and Development of a Ventilator Exhaust Pathogen Deactivation Technology Using Advanced Manufacturing Techniques

TOTAL APPROVED AMOUNT:
$80,000 over less than 1 year

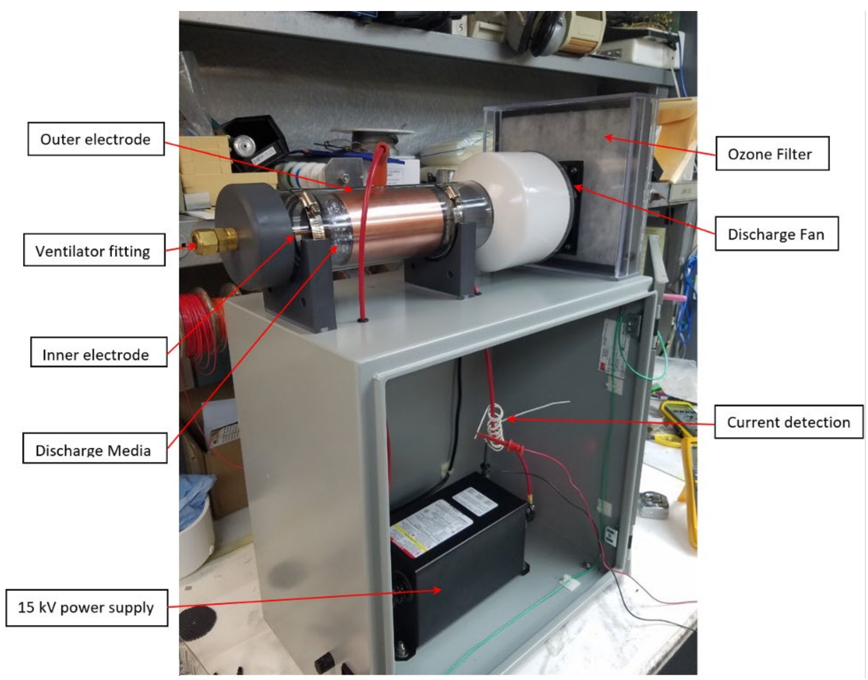
PROJECT NUMBER:
20A1051-003

PRINCIPAL INVESTIGATOR:
A. Andy Beasley, INL

CO-INVESTIGATORS:
Randy Bewley, INL
Mark DeHart, INL
Richard Hatch, INL
Dennis James, INL
Eric Lumley, INL
Michael McMurtrey, INL
Patrick Moo, INL
Robert O'Brien, INL
Amanda Smolinski, Idaho State University

Researchers responded quickly to rapidly prototype a sterilizer for medical ventilators adaptable to advanced manufacturing techniques to provide a low-cost, scalable solution to the problem of high-efficiency particulate air (HEPA) filters on ventilators plugging with high volumes of mucous, as seen in COVID-19 patients.

INL researchers responded to a specific need related to the COVID-19 pandemic and improved the functionality of medical ventilator units by eliminating the outlet HEPA filter, which can become plugged with moisture from mucous discharges seen in COVID-19 patients. The sterilizer uses a non-thermal plasma generated by high voltage coronal discharge in a reaction chamber to inactivate the virus. The design of the sterilizer makes it more tolerant of moisture than the traditional HEPA filter, thereby reducing or eliminating filter replacements and reducing medical staff workload. This type of low cost, replaceable reaction chamber that inactivates pathogens can reduce the exposure of room occupants, particularly medical staff, to infectious agents. The prototype proves the efficacy of a future deployable sterilizer authorized under a U.S. Food and Drug Administration emergency use authorization.



Prototype of a sterilizer for medical ventilators developed using off-the-shelf components.

Development of Advanced 3D Printing Technologies for Cutting Edge Materials

TOTAL APPROVED AMOUNT:
$804,100 over 3 years

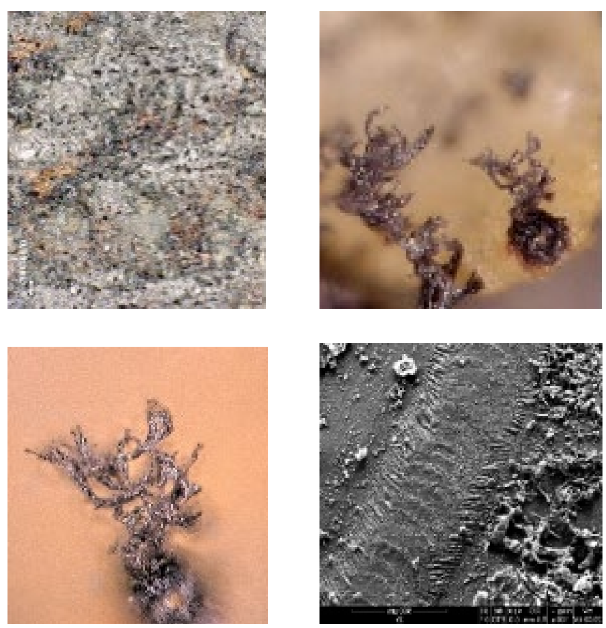
PROJECT NUMBER:
18A12-130

PRINCIPAL INVESTIGATOR:
Colt Heathman, INL

CO-INVESTIGATORS:
Edna Cardenas, INL
Alexander May, INL
Rocklan McDowell, INL

Researchers identified novel precursor materials for use as feed materials in 3D printers to develop advanced 3D printing technologies for cutting edge materials.

Innovations in advanced materials and manufacturing are supporting technologies deployed under extreme or harsh environments, including high-radiation fields, temperature extremes, corrosive species, chemical containment, dynamic loading, mechanical impact, and both vacuum and high-pressure atmospheres. In particular, the ability to use feed materials beyond metallic powders, such as oxides or metal chelates that readily undergo decomposition, to deposit the metallic metal or ceramic forms shows considerable promise for additive manufacturing in the nuclear and national security spaces. To develop advanced 3D printing technologies for cutting edge materials, researchers identified novel precursor materials for use as feed materials in 3D printers such as the OPTOMEC laser-engineered net shaping (LENS™) 3D printer. Then, they developed metal complex powders suitable for additive manufacturing with suitable pyrolysis and/or combustion properties to reduce to the metallic state. After powder preparation, the powder was converted through laser welding tests where conversion of metal-complex materials was observed. Developing novel metal complex powders addresses the head end of additive manufacturing (AM) to broaden the applicability of additive manufacturing to harsh and extreme environments beyond the use of conventional materials.



Bulk zirconium acetylacetonate ($Zr(AcAc)_4$) after laser welding under limited conditions (top left). Conversion boundary of neat $Zr(AcAc)_4$ (top right). Zoomed-in image of the tree-like structure shown in the conversion boundary area (bottom left). Scanning electron microscope image of welded $Zr(AcAc)_4$ on zirconium backing plate (bottom right).

Electrochemical Co-production of Ammonia and Ethylene Using Ethane and Nitrogen at Intermediate Temperature (300-450 °C)

TOTAL APPROVED AMOUNT:
$676,700 over 2 years

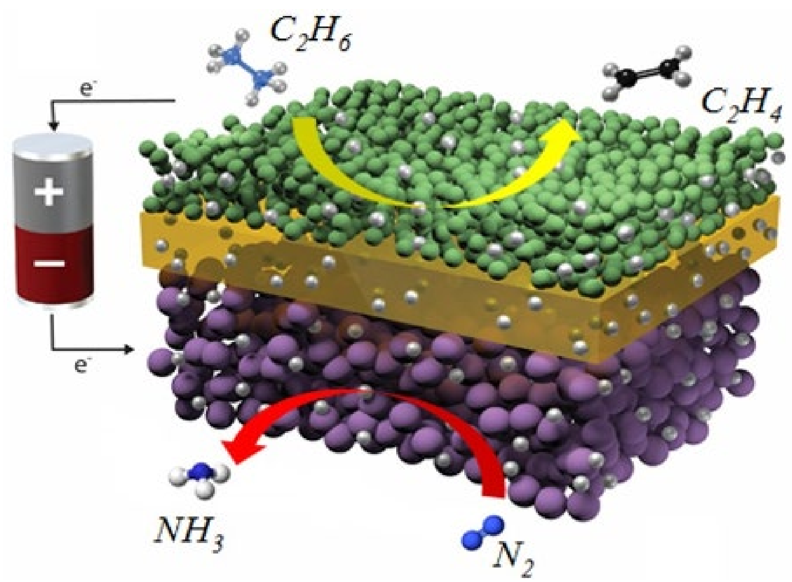
PROJECT NUMBER:
19A39-126

PRINCIPAL INVESTIGATOR:
Dong Ding, INL

CO-INVESTIGATORS:
Rebecca Fushimi, INL
Lucun Wang, INL

Researchers designed and developed a novel process to co-produce ammonia and ethylene through a disruptive electrochemical approach using natural gas/natural gas liquids and nitrogen as the feedstock at intermediate temperatures.

This project included the design and development of novel nitrogen reduction reaction catalysts and the evaluation of combined catalysts and thermally-stable ceramic proton-conducting membrane. The current understanding of transition metal catalysis indicates that the electronic structure is central to the activity with the topmost atomic layers of catalyst playing an important role in the mechanism and kinetics of catalytic reactions, meaning that they can be easily tuned by appropriate design of synthesis process. Using this understanding as a starting point, researchers synthesized and evaluated the performance of a series of cerium-ruthenium-based catalysts for ammonia synthesis reaction under ambient pressure in both a fixed-bed flow reactor and an electrochemical membrane reactor. A Temporal Analysis of Products reactor system experiment was also employed to understand the mechanistic aspects of ammonia synthesis over catalyst. This new process enables and informs future innovation in the petroleum chemical industry as well as in nuclear heat and electricity utilization.



Evaluation of combined catalysts and thermally stable ceramic proton-conducting membrane.

TALENT PIPELINE:

Postdocs:

- Bin Hua, INL
- Meng Li, INL
- Yixiao Wang, INL

Students:

- Joshua Gomez (GEM Fellow), New Mexico State University
- Wei Tang, New Mexico State University

INTELLECTUAL PROPERTY:

One U.S. patent application filed (16/532,276): Methods and Systems for Co-Producing Hydrocarbon Products and Ammonia, and Related Electrochemical Cells

Two U.S. provisional patent applications filed (BA-1180P; BA-1216P): A Sustainable Electrochemical Process for Ammonia Synthesis Using Greenhouse Gases; Tuning the Size Regime of Supported Metal Nanomaterials

PUBLICATIONS:

Cao, Z., Z. Song, F. Liang, X. A., K. K. Al-Quraishi, M. Wang, J. Chen, D. Ding, and Y. Yang. 2020. "Hydrogen Bonding Sewing Interface." RSC Advances 10(30): 17438-13443. https://doi.org/10.1039/D0RA00366B.

Ding, H., W. Wu, and D. Ding. 2019. "Advancement of Proton-Conducting Solid Oxide Fuel Cells and Solid Oxide Electrolysis Cells at Idaho National Laboratory (INL)." ECS Transactions. 91(1): 1029-1034. https://doi.org/10.1149/09101.1029ecst.

Gao, S., R. Wang, C. Ma, Z. Chen, Y. Wang, M. Wu, Z. Tang, N. Bao, D. Ding, W. Wu, F. Fan, and W. Wu. 2019. "Wearable high-dielectric-constant polymer with core-shell liquid metal inclusions for biomechanical energy harvesting and self-powered user interface." Journal of Materials Chemistry A. 7(12) 7109-7117. https://doi.org/10.1039/C9TA01249D.

Li, M., B. Hua, L.-C. Wang, J. Sugar, W. Wu, Y. Ding, J. Li, D. Ding. Accepted for publication in 2021. "Switching of metal-oxygen hybridization for selective CO_2 electrohydrogenation under mild temperature and pressure." Nature Catalysis.

Tang, W., J. Jian, G. Chen, W. Bian, J, Yu, H. Wang, M. Zhou, D. Ding, and H. Luo. 2020. "Carbon-nanotube Supported MoS_2 via Microwave-Heating for Enhanced Performance of Hydrogen Evolution." Energy Materials Advances 2021:8140964. https://doi.org/10.34133/2021/8140964.

Wang, H., X. Chen, D. Huang, M. Zhou, D. Ding, and H. Luo. "Cation Deficiency Tuning of $LaCoO_3$ Perovskite as Bifunctional Oxygen Electrocatalysts." ChemCatChem 12 (10): 2768-2775. https://doi.org/10.1002/cctc.201902392.

Wang, H., L. Yan, T. Nakotte, W. Xu, M. Zhou, D. Ding, and H. Luo. 2019. "IrO_2-incorporated $La_{0.8}Sr_{0.2}MnO_3$ as Bifunctional Oxygen Electrocatalysts with Enhanced Activities." Inorganic Chemistry Frontiers 6(4): 1029-1039. https://doi.org/10.1039/C9QI00033J.

Wang, L.-C., Y. Zhang, J. Xu, W. Diao, S. Karakalos, B. Liu, X. Song, W. Wu, T. He, and D. Ding. 2019. "Non-oxidative Dehydrogenation of Ethane to Ethylene over ZSM-5 Zeolite Supported Iron Catalysts." Applied Catalysis B: Environmental 256: 117816. https://doi.org/10.1016/j.apcatb.2019.117816.

Xu, W., N. Apodaca, D. Ding, L. Yan, G. Chen, M. Zhou, P. Choudhury, and H. Luo. 2019. "A-site Excessive $(La_{0.8}Sr_{0.2})_{1.05}MnO_3$ and $(La_{0.8}Sr_{0.2})_{1.1}MnO_3$ Perovskite Oxides for Bifunctional Oxygen Catalyst in Alkaline Media." ACS Catalysis 9(6): 5074-5083. https://doi.org/10.1021/acscatal.9b00800.

Ye, R.-P., L. Lin, L.-C Wang, D. Ding, Z. Zhou, P. Pan, Z. Xu, J. Liu, H. Adidharma, M. Radosz, and M. Fan. 2020. "Perspectives on the Active Sites and Catalyst Design for the Hydrogenation of Dimethyl Oxalate." ACS Catalysis 10(8):4465-4490. https://doi.org/10.1021/acscatal.9b05477.

Surface Morphological Patterning, Structure-activity Modeling, and Aging Analysis of Catalyst Materials to Enhance Oxidative Dehydrogenation of Ethane Reaction Conversion Efficiency

TOTAL APPROVED AMOUNT:
$805,300 over 3 years

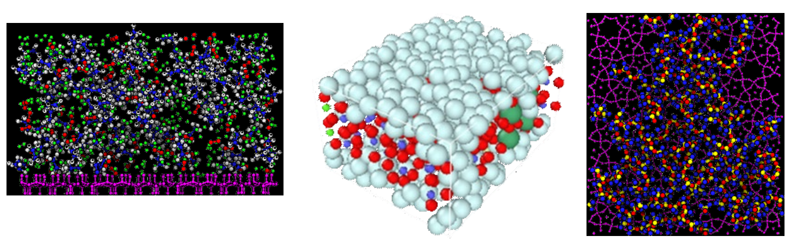
PROJECT NUMBER:
18A12-210

PRINCIPAL INVESTIGATOR:
Kevin Gering, INL

CO-INVESTIGATORS:
Eric Jankowski, Boise State University
Matthew Jones, Boise State University
Jeffrey Rimer, University of Houston
Chase Taylor, INL
Jagoda Urban-Klaehn, INL

To improve catalyst design and use conditions, researchers developed inroads to understanding catalyst fate and performance through a diverse approach comprised of large-scale surface modeling based on GPU, positron-based diagnostics, precise laboratory aging of catalysts, and a diagnostic and predictive modeling approach based on periodic transient cycling (catalytic or electro-catalytic) that renders catalyst surface deactivation over several hundred cycles.

This research addressed three critical aspects of catalysts: performance, diagnostics, and aging. In terms of performance, researchers chose oxidative dehydrogenation of ethane as an important example route toward ethylene production, using an M1-type catalyst composed of blended transition metal oxides. Computational work employed GPU-based methods to gain knowledge on structure-activity relationships as they pertain to M1 surface augmentation (chemical masking) to improve catalyst selectivity and surface diffusion of key reactants to better facilitate oxidative dehydrogenation of ethane. Diagnostics of aged or deactivated zeolite catalysts were facilitated by positron-based techniques. Zeolite Socony Mobil–5-type samples were used that had experienced different stages of aging while under methanol-to-hydrocarbons conditions. An additional modeling framework was developed that evaluates catalyst deactivation over a host of reaction conditions using a transient analysis basis. Key impacts are seen in the computational and experimental methods that speak to the needs within the larger industry that depend on catalysts. This work enables guiding design, diagnose and operate more efficient and selective catalysts, as well as key knowledge on catalyst usage pathways that can be optimized to reduce aging and the associate cost of catalyst replacement.



An example M1 surface simulation (side-on view) containing gas of 15% ethane, 10% oxygen, 75% helium by moles. Red = oxygen, blue = carbon, white = hydrogen, green = helium, and the magenta = M1 surface (left); unit M1 crystalline cell sandwiched by high-pressure gas mixture containing ethane, oxygen and helium (center); and M1 surface simulation including the poly(dimethyl siloxane) polymeric patterning agent. The poly(dimethyl siloxane) is aggregating, leading to the blocking of particular regions of the M1 crystal while leaving other regions free to perform oxidative dehydrogenation (right).

TALENT PIPELINE:

Students:

- Mike Henry, Boise State University
- Thuy Thanh Le, University of Houston
- Neale Ellyson, Boise State University
- Mone't Alberts, Boise State University
- Bryton Anderson, Boise State University
- Chris Jones, Boise State University
- Mitchell Leibowitz, Boise State University

PUBLICATIONS:

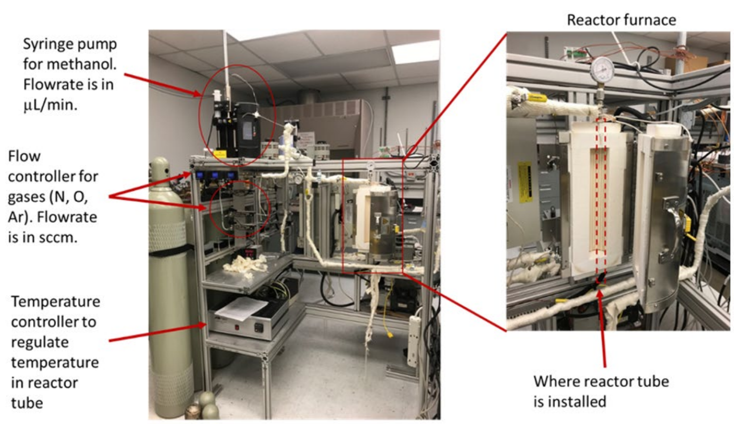
Jankowski, E., N.Ellyson, J. W. Fothergill, M. M. Henry, M. H. Leibowitz, E. D. Miller, M. Alberts, S. Chesser, J. D. Guevara, C. D. Jones, M. Klopfenstein, K. K. Noneman, R. Singleton, R. A. Uriarte-Mendoza, S. Thomas, C. E. Estridge, and M. L. Jones. 2020. "Perspective on Coarse-graining, Cognitive Load, and Materials Simulation." Computational Materials Science. 171:109129. https://doi.org/10.1016/j.commatsci.2019.109129.

Urban-Klaehn, J.M., K.L. Gering, C.N. Taylor, and C.A. Quarles, 2020. "Positron Parameters for Atypical Samples." Acta Physica Polonica A 137, no. 2: 201. https://doi.org/10.12693/APhysPolA.137.201.

PRESENTATIONS:

Taylor, C.N., T.F. Fuerst, and M. Shimada. 2019. "Characterization of Coincidence Doppler Broadening and Positron Annihilation Lifetime Systems at INL." AIP Conference Proceedings 2182(1): 040010.https://doi.org/10.1063/1.5135842.

Urban-Klaehn, J., K.L. Gering, and D. Miller. 2019. "Doppler Broadening Spectroscopy Used as Kapton Thickness Sensor, AIP Conference Proceedings 2182(1): 050019. https://doi.org/10.1063/1.5135862.



Laboratory set-up of packed-bed reactor for heterogeneous catalyst testing at the University of Houston. A typical set-up includes flow controllers, syringe pump for reactant, and temperature controller for the reactor furnace.

Multi-scale Modeling and Optimization of Additive Manufacturing Process for Nuclear Fuels

TOTAL APPROVED AMOUNT:
$487,300 over 2 years

PROJECT NUMBER:
19A39-067

PRINCIPAL INVESTIGATOR:
Wen Jiang, INL

CO-INVESTIGATORS:
Yipeng Gao, INL
Subhashish Meher, INL
Jeong-Hoon Song,
University of Colorado, Boulder
Isabella Van Rooyen, INL
Congjian Wang, INL
Xu Wu, North Carolina State University

A new MOOSE-based application called Valhalla models all the steps of an AM process across multiple length scales.

Compared to traditional fuel production techniques, AM techniques greatly reduce the production time and cost and provide flexibility to nuclear fuel design for better performance. Despite the advantages, these AM techniques need to be optimized due to defects from highly complex melting and sintering process. The complex metallurgical phenomena during AM are strongly related to the relevant AM process parameters such as applied laser power, traveling speed and scan style, which could lead to differences in density, residual stress, crystallographic texture, and mechanical properties. Modeling and simulation become highly attractive to support optimal AM process development and fundamentally understand the various physical interactions and process sensitivities. This project developed a new MOOSE-based application called Valhalla to model all steps of the AM process across multiple length scales. At macroscale, a finite element analysis workflow was implemented to simulate directed energy deposition AM process and to predict thermal conditions, residual stress, and distortion during manufacturing. At mesoscale, a multi-physics model was developed to model highly nonlinear phenomenon including heat transfer, melting, and fluid flow in melt pool. At microstructure level, a phase-field model was developed to simulate alloy solidification during AM process. Phase-field modeling was also performed to investigate the effects of existing pores produced during AM on irradiated materials. Inverse uncertainty quantification under the Bayesian framework was utilized to build a relation between uncertain inputs, model prediction, and experimental data. To facilitate optimization, gaussian processes and physics-informed neural networks were employed for surrogate models of the expensive finite element modeling. Valhalla, the resulting MOOSE-based application, can produce macroscale finite element analysis of AM processes and perform melt pool dynamics simulation which integrates meso-scale phase-field modeling of alloy solidification. The comprehensive modeling framework developed by this project applies directly to reactor fuel design, fabrication, and modeling, as well as to modeling metals, ceramics, and composites for other fossil and renewable energy applications.

TALENT PIPELINE:

Postdoc:

- Dewen Yushu, INL

Student:

- Feiyang Chen, Clemson University

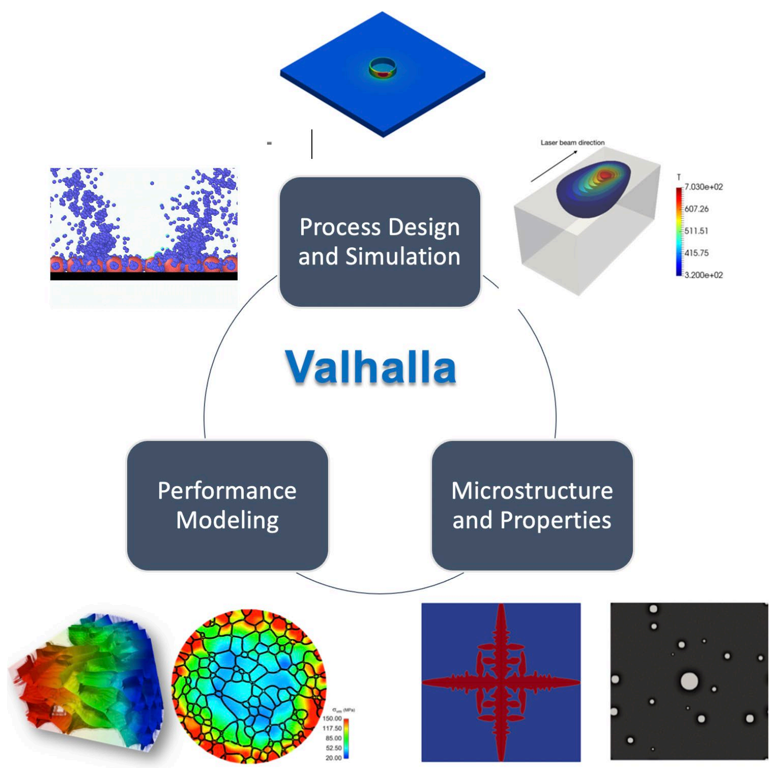
PUBLICATIONS:

Almasi, A., A. Beel, T.Y. Kim, J. G. Michopoulos, and J.H. Song. 2019. "Strong-form Collocation Method for Solidification and Mechanical Analysis of Polycrystalline Materials." Journal of Engineering Mechanics, 145(10): 04019082. https://doi.org/10.1061/(ASCE)EM.1943-7889.0001665.

Almasi, A., T.Y. Kim, and T. A. Laursen, and J.H. Song. 2019. "A Strong Form Meshfree Collocation Method for Frictional Contact on a Rigid Obstacle." Computer Methods in Applied Mechanics and Engineering 357: 112597. https://doi.org/10.1016/j.cma.2019.112597.

PRESENTATION:

Wang, C., W. Jiang, and Y. Gao, "Modeling Time-dependent Surrogates of Additive-manufactured Nuclear Fuels Processes." Transactions of the American Nuclear Society 122, no. 1 (Virtual Conference June 8-11): 272-275. https://dx.doi.org/10.13182/T122-32604.



Valhalla is a MOOSE-based application of multi-scale modeling of an additive manufacturing process.

On-demand Olefin Separations Using Facilitated Transport Membranes

TOTAL APPROVED AMOUNT:
$125,000 over 1 year

PROJECT NUMBER:
20A1049-013

PRINCIPAL INVESTIGATOR:
John Klaehn, INL

CO-INVESTIGATORS:
Glenn Lipscomb, University of Toledo
Christopher Orme, INL

Researchers made significant progress towards creating a unique facilitated transport membrane demonstrated for high ethylene production that is implemented with electrochemical non-oxidative deprotonation which will be used in integrated energy systems.

Alternative strategies are needed to increase efficiencies in integrated energy systems, including finding new applications for heat and electricity during periods of overgeneration. One option is new hydrophobic polymer membranes for ethylene/ethane separations that can be utilized in electrochemical non-oxidative deprotonation (ENDP). ENDP produces ethylene by electrochemical dehydrogenation of ethane without needing water vapor during its operation. The separation of ethylene, an olefin, from ethane by polymer membranes is extremely difficult due to both gases have similar molecular sizes and boiling points. Therefore, a facilitated transport mechanism is the only viable option for this separation. In this case, facilitated transport membranes (FTMs) use a molecular species that has affinity for olefins and acts as a shuttle for olefins through the polymeric matrix. To advance the goal, fabricating FTMs, polymer benchmarking, FTM fabrication, and FTM characterization were completed on several highly permeable polymers for ethylene separation. Two aspects of the FTM were explored: 1) ethylene facilitators and 2) highly permeable hydrophobic polymer. Silver salts showed the best ethylene facilitation, and they were used for FTM fabrication and analyses. Several highly permeable hydrophobic polymers were analyzed for their gas permeability measurements. Some polymers with high permeabilities included polydimethylsiloxane, poly(1-trimethysilyl)-1-propyne, and polymer of intrinsic microporosity. These polymers were tested and their ethylene permeabilities are above 1000 Barrers. One polymer with silver facilitator showed excellent permeability and selectivity for ethylene over ethane. These results inform new, custom designed FTM modules for various industrially relevant applications, such as ENDP.

TALENT PIPELINE:
Student:

- Arsalan Sepehri, University of Toledo

Poly(1-trimethysilyl)-1-propyne membranes were created and tested and showed ethylene permeabilities are above 1000 Barrers. Poly(1-trimethysilyl)-1-propyne with silver facilitator is being developed to determine if it can achieve better ethylene permeability.

Ontology for the Design of Innovative Nuclear Technologies

TOTAL APPROVED AMOUNT:
$129,500 over 1 year

PROJECT NUMBER:
19A42-024

PRINCIPAL INVESTIGATOR:
Christopher Ritter, INL

CO-INVESTIGATORS:
Mikhail Auguston, Naval Postgraduate School
Jeren Browning, INL
Kristin Giammarco, Naval Postgraduate School
Anthony Pollman, Naval Postgraduate School
Mark Stevens, Naval Postgraduate School
Douglas Van Bossuyt, Naval Postgraduate School
Clifford Whitcomb, Naval Postgraduate School

A new nuclear ontology is the first fully open-source common ontology for nuclear design with a scientific basic formal ontology core that allows for standardization of a data model for reactor design with verification and validation of the data model's functional properties facilitated through modeling and simulation.

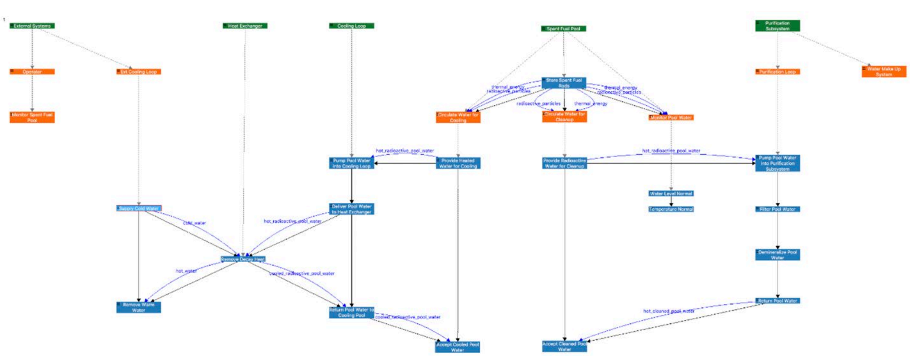
The construction, aerospace, and automotive industries have achieved considerable cost and schedule savings by utilizing virtual design. This approach is not shared by the nuclear industry where the current ecosystem of tools and solutions for nuclear technology development implement proprietary data ontologies to capture design information. The storage of critical design information is in disparate, proprietary systems which reduces the ability to connect information. To create a generic, common framework to enable digital engineering programs for reactor design, this project developed a formal representation of information called a data ontology. A usable ontology needed to be compatible with other domain ontologies, right sized to ensure the ontology is deep enough to be useful but flexible enough to support multiple designs and verified to ensure that functional specifications are executable. These parameters were met through analysis and selection of top level meta models, followed by the development of lower ontological decompositions for nuclear design using subject matter input to create an easily extendable ontology framework, and the validation and verification of the ontology for nuclear reactor behavior models using Monterey Phoenix. The resulting Data Integration Aggregated Model for Nuclear Deployment (DIAMOND) nuclear ontology empowers the development of innovative nuclear technologies by facilitating the development of a single digital engineering platform to support multiple nuclear energy programs, saving costs, and encouraging collaboration.

TALENT PIPELINE:
Students:

- Matthew Ball, North Carolina State University
- Joel Corporan, Georgia Institute of Technology (Georgia Tech)
- Chara Robertson, North Carolina Agricultural and Technical State University
- Arkasia Wyatt, Norfolk State University

INTELLECTUAL PROPERTY:
One software copyright filed (CW-19-19): DIAMOND, available open source on GitHub: https://github.com/idaholab/DIAMOND.

PRESENTATION:
Ritter, C., J. Browning, L. Nelson, T. Borders, J. Bumgardner, and M. Kerman. 2020. "Digital Engineering Ecosystem for Future Nuclear Power Plants: Innovation of Ontologies, Tools, and Data Exchange. Presented at the 18th Annual Conference on Systems Engineering Research (CSER) (Virtual Conference Oct. 08-10).



Nominal behavior of spent fuel cooling pool (Monterey Phoenix event trace). Green boxes are root events (actors), orange boxes are composite events, and blue boxes are atomic events.

Thermomechanical Processing of Titanium Alloys for Improved Ballistic Performance

TOTAL APPROVED AMOUNT:
$610,500 over 3 years

PROJECT NUMBER:
18A12-088

PRINCIPAL INVESTIGATOR:
Thomas Lillo, INL

CO-INVESTIGATORS:
Jeffrey Anderson, INL
K. Ryan Bratton, INL
Henry Chu, INL
Jason Walleser, INL

COLLABORATOR:
Denis Clark, DECLark Welding Engineering

A methodology was developed to rapidly identify deformation processing parameters suitable to form the target alloy into a useful component.

The physical protection R&D community needs a more cost-effective, science-based approach to accelerate development of new alloys for armor applications, especially lightweight armor applications and other extreme environment applications. Computational alloy-by-design methods accelerate alloy discovery; however, final mechanical properties are strongly influenced by the thermomechanical processing (TMP) schedule used to form the alloy into a useful component with the requisite properties. Currently, TMP schedule development of new armor alloys, as well as alloys for other extreme environment applications, is based on an expert-based, trial-and-error process, which is both time-consuming and costly. Accelerating optimization of the TMP pathway can yield optimal microstructure, mechanical properties, and maximum ballistic performance.

Researchers developed a methodology to rapidly identify deformation processing parameters, such as hot forming temperatures and forming strain rates, suitable to form the target alloy into a useful component. Subsequently, the optimum, post-forming heat treatment schedule to obtain optimum application-specific performance was rapidly identified using an artificial intelligence approach and an advanced design-of-experiments approach. The approach reduced experimental testing by >90% while adequately covering the heat treatment parameter space. Development and demonstration of the approach was carried out on titanium alloy ($Ti_{10}V_2Fe_3Al$) that was originally developed for aircraft landing gear. However, utilizing this high-strength, low density alloy for ballistic protection applications requires a different combination of mechanical properties compared to aircraft landing gear applications, and thus required a different TMP processing schedule which researchers investigated as a demonstration of the TMP optimization approach. Ultimately, the approach was demonstrated to be effective in hot rolling 50 mm thick $Ti_{10}V_2Fe_3Al$ plate down to 17 mm thick to produce panels for ballistic testing. Subsequently, an artificial intelligence-based approach was developed to establish the post-processing heat treatment parameter/mechanical property relationship, which is being applied to the rolled $Ti_{10}V_2Fe_3Al$ plates to be used in ballistic tests. These results prove that applying a science-based approach to armor alloy development reduces cost and time-to-deployment.

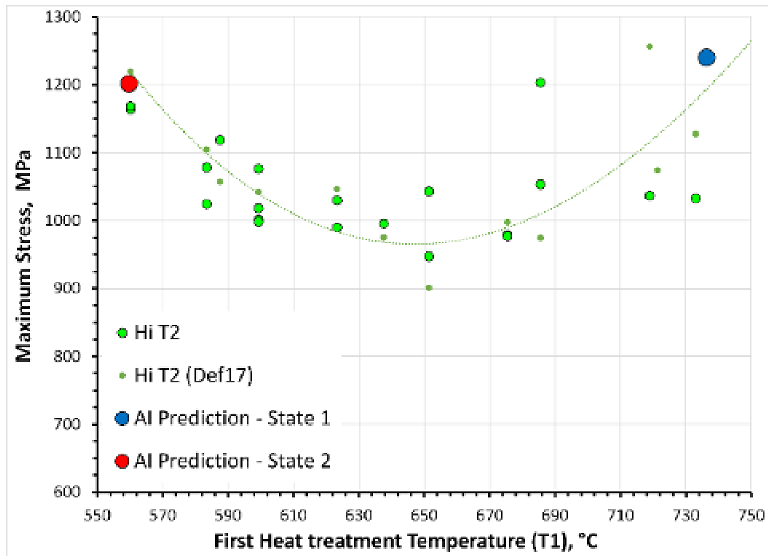
TALENT PIPELINE:

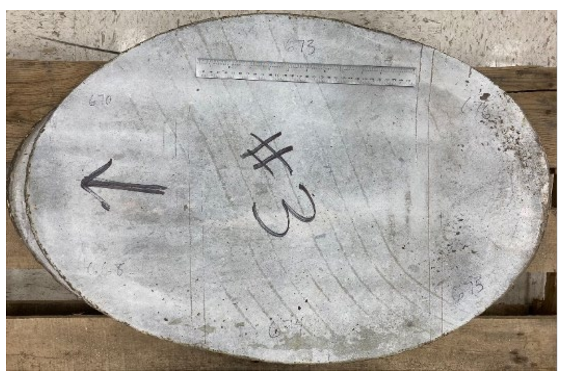
Student:

- Chad Matthews, Colorado School of Mines

PRESENTATION:

Lillo, T., H. Chu, J. Anderson, J. Walleser, and V. Burguess. 2019. "Rigorous Accelerated Approach to Thermomechanical Processing Optimization for New Ballistic Protection Alloys." Proceedings of the Ground Vehicle Systems Engineering and Technology Symposium (GVSETS), NDIA (Novi, MI, Aug. 13-15). http://gvsets.ndia-mich.org/documents/MAM/2019/ThermomechanicalProcessingOptimization_Lillo_Thomas_619 2019.pdf.





AI predictions of heat treatment parameters needed and successfully rolled $Ti_{10}V_2Fe_3Al$ plate using those parameter predictions to maximize the ultimate strength.

In today's interconnected world a subtle risk can rapidly evolve into a major threat. Researchers at INL are dedicated to the physical and cyber security of the critical assets, control systems, and operational technology of our nation's critical infrastructure.

SECURE AND RESILIENT CYBER-PHYSICAL SYSTEMS

Today's threat environment requires inherently secure and resilient cyber-physical systems for all critical infrastructure, including energy systems. INL advances automated-control solutions for vital systems and critical infrastructure through its well-established control systems cybersecurity capability. The combination of INL's threat analysis and consequence-based risk prioritization with embedded, component, and system security RD&D for critical process technology propels the development of automated threat responses and resilient systems that limit the physical effects of cyberattacks. Through the secure and resilient cyber-physical systems S&T initiative, INL develops new cyber-informed engineering methods and technologies for automated controls that are validated systematically at scale.

Finding the Origins of a Hacker

Sarah Freeman, a senior industrial control systems cybersecurity analyst at INL, is focused on critical infrastructure protection and works to protect the industrial control systems that run utilities from attacks via malicious code. Freeman's work, funded by a Seed LDRD award, addressed the "who" of a potential cyberattack by putting together a series of clues to determine who is behind an attack, which allows the government to potentially act against known perpetrators. Freeman noted that working through all of these possibilities of "what," "why," and "how" to ascertain "who" is difficult, but her research on the challenges of cyber attribution is aimed at making such a forensic analysis of an attack more thorough.

Sarah Freeman's ongoing work in cyber attribution started with an LDRD project.

CyPhy: Cyber-secure Physical Layer Security in Millimeter Wave (mmWave) Communications

TOTAL APPROVED AMOUNT:
$884,800 over 3 years

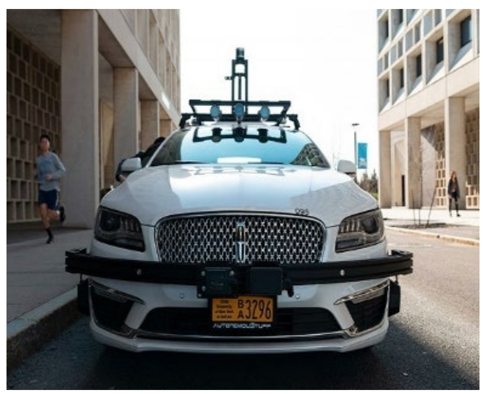
PROJECT NUMBER:
18A12-131

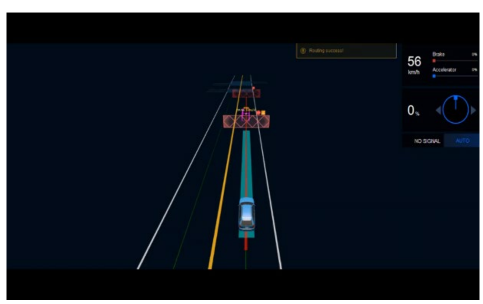
PRINCIPAL INVESTIGATOR:
Arupjyoti Bhuyan, INL

CO-INVESTIGATORS:
Zhi Sun, State University of New York at Buffalo
Pu Wang, University of North Carolina, Charlotte

Researchers concluded that communications can be effectively protected from eavesdropping and cyber intrusion with mmWave physical layer designed-in security features.

It is expected that billions of fifth generation (5G) mobile and Internet of things wireless devices will be all connected in the mmWave frequency bands. This necessitates development of technology to secure delivery of information during wireless transmissions that are susceptible to the increasing computational capabilities of unauthorized devices. Researchers had four objectives for this project: 1) identifying and analyzing physical layer features that are unique to the wireless devices used for 802.11ad mmWave communication systems; 2) extracting unique beam pattern features to distinguish end devices with a convolutional neural network; 3) extracting unique radiofrequency biometric signatures using a customized residual deep neural network; and 4) tracking and recognizing with an active mmWave system using customized residual deep neural network. The resulting innovative secure wireless system, called CyPhy, with novel physical layer security capabilities achieves cyber security in mmWave communications, enhancing cyber security, protection, and assurance of advanced wireless communications, building expertise in secure mmWave connectivity for 5G and Internet of things, expanding wireless research portfolio for critical infrastructure protection, and ensuring national security.





A Lincoln MKZ car equipped with mmWave radar was used to collect real world data from test drives, and then attacks were simulated using the Apollo Baidu platform for scenarios, including spoofed appearance of stalled vehicles and hard braking by an autonomous vehicle.

TALENT PIPELINE:

Student:

- Prabhu Janakaraj, University of North Carolina, Charlotte

INTELLECTUAL PROPERTY:

One U.S. provisional patent application filed (62/868,062): Systems, Devices, and Methods for Authenticating Millimeter Wave Devices

PUBLICATIONS:

Balakrishnan, S., S. Gupta, A. Bhuyan, P. Wang, D. Koutsonikolas, Z. Sun. 2019. "Physical Layer Identification Based on Spatial-temporal Beam Features for Millimeter Wave Wireless Networks." IEEE Transactions on Information Forensics & Security 15: 1831-1845. https://doi.org/10.1109/TIFS.2019.2948283.

Balakrishnan, S., P. Wang, A. Bhuyan, and Z. Sun. 2019. "Modeling and Analysis of Eavesdropping Attack in 802.11ad mmWave Wireless Networks." IEEE Access 7: 70355-70370. https://doi.org/10.1109/ACCESS.2019.2919674.

PRESENTATION:

Balakrishnan, S., P. Wang, A. Bhuyan, and Z. Sun. 2019. "Impact Analysis of Mobility on Physical Layer Security of mmWave Networks." 2019 Resilience Week: 163-168. https://doi.org/10.1109/RWS47064.2019.8971814.

INL's wireless test bed, including fixed and mobile towers spread across the 890 square-mile desert site, facilitates full-scale testing and demonstration of wireless systems and equipment.

Establishing Metrics for Measuring Firmware Construction Quality

TOTAL APPROVED AMOUNT:
$315,000 over 2 years

PROJECT NUMBER:
19A39-056

PRINCIPAL INVESTIGATOR:
Robert Erbes, INL

COLLABORATORS:
Cyber Independent Testing Lab
Red Balloon Security

Researchers developed independent, scalable, repeatable, and automated analysis of firmware used in both critical infrastructure and commodity devices that could inform vendors and utility consumers as to where products stand with regards to implementation of existing security technologies.

Currently, the only method for a consumer to independently evaluate the security and quality of software is a quantitative evaluation method under development by the Cyber Independent Testing Lab. Beyond this effort, there is a significant gap in options for consumers to independently evaluate the security and quality of software. This project sought to develop a reliable way to evaluate the security and quality of firmware, the underlying, low-level software that interfaces directly with hardware in computer equipment, especially the firmware on devices that run the nation's critical infrastructure and industrial control systems (ICS). A large sample of firmware from ICS devices was collected and analyzed, consisting of extraction from physical devices and downloading firmware from vendors that made their firmware available online. Results from this analysis show that the ICS industry has fallen behind in utilizing existing security technologies. The state of the secure coding and implementation practices used by ICS vendors (with emphasis on devices deployed for energy) indicates that ICS vendors are not performing significantly better than counterparts in the information technology and Internet of things sectors. Researchers are collaborating with Cyber Independent Testing Lab and Red Balloon Security to make these results known to vendors and consumers to inform improved best practices for firmware in ICS and critical infrastructure.

INL researchers collaborated closely with industry to establish that independent vulnerability analysis and reporting are important tools for overall industrial control system security in an environment where vendors are still not achieving basic cyber security baselines in their products.

Electric Vehicle Wireless Charging Security

TOTAL APPROVED AMOUNT:
$642,100 over 3 years

PROJECT NUMBER:
18A12-070

PRINCIPAL INVESTIGATOR:
Kenneth Rohde, INL

CO-INVESTIGATORS:
Barney Carlson, INL
Abhilash Kamineni, Utah State University
Regan Zane, Utah State University

Researchers performed a cyber security assessment on a commercially available wireless power transfer (WPT) system used in electric vehicles revealing potential areas of concern.

The security and reliability of electric vehicle wireless charging communication systems is potentially vulnerable to manipulation or alteration which can result in unintended consequences such as lack of proper functionality, potential safety hazards, and even disruptions to the electric grid. Advancing the study of WPT systems by assessing potential vulnerabilities and researching functional capabilities before these charging stations become prevalent will help protect both individual vehicles and charging stations and national energy infrastructure more broadly. Researchers investigated the security posture of various WPT wireless communications and analyzed various power electronic components and electromagnetic-field safety systems for reliability during loss or manipulation of control communications. In addition to identifying and analyzing cyber security vulnerabilities and power engineering issues in a WPT system, researchers also examined dynamic WPT, or in-motion vehicle charging. These assessments revealed a severe lack of proper cyber hygiene practices as well as the use of proprietary wireless communications that do not adhere to the currently proposed recommended practice. Results of these assessments inform engineering research, modeling, and simulation to better design WPT and dynamic WPT systems to ensure their security.

PUBLICATION:

Bagchi, A.C., A. Kamineni, R. Zane, and R. B. Carlson. 2021. "Review and Comparative Analysis of Topologies and Control Methods in Dynamic Wireless Charging of Electric Vehicles." IEEE Journal of Emerging and Selected Topics in Power Electronics (Feb.). https://doi.org/10.1109/JESTPE.2021.3058968.

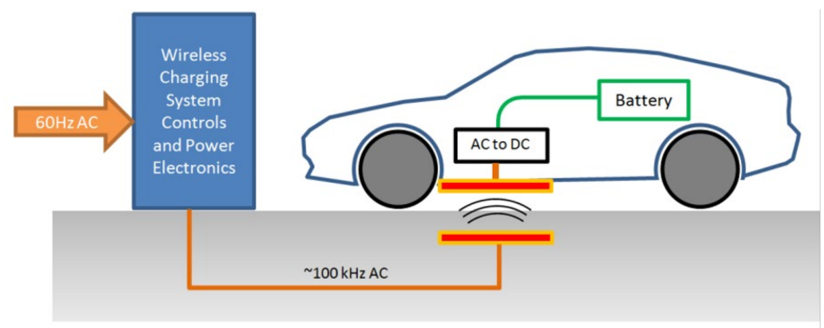


Illustration of wireless charging system interface with an electric vehicle.

Dynamics of Multi-layer Complex Infrastructure Networks

TOTAL APPROVED AMOUNT:
$454,600 over 3 years

PROJECT NUMBER:
18A12-132

PRINCIPAL INVESTIGATOR:
Ryan Hruska, INL

CO-INVESTIGATOR:
Iris Tien, Georgia Tech

Researchers modeled critical infrastructure systems as complex and interdependent networks, allowing for dynamic analysis of the resilience and robustness of these connected systems and a quantitative assessment of the risk and resilience of mutually dependent infrastructure systems.

Critical infrastructure is ubiquitous in modern societies and their reliable and resilient operation is of paramount importance to national security and economic vitality. Recent trends have been to optimize the operation of these systems, which have resulted in the tight coupling of both their physical and cyber components. It is important to develop a better understanding of the behavior of the resulting complex interdependent infrastructure networks to better estimate the reliability and resiliency of real-world infrastructure systems under adverse conditions. This need has been repeatedly reinforced by events such as the 2003 Northeast Blackout, 2012 Superstorm Sandy, and the 2021 Texas Polar Vortex which all resulted in significant impacts. This research advanced the ability to evaluate how scale, time, and structure influence the behavior of individual infrastructure networks as well as the resulting complex multilayered network. The novel approach applied in this project included synthetic generation of infrastructure networks with machine learning, graph representations that capture maximum dynamics of complex networks, and novel analytic techniques to measure resilience and robustness of interconnected networks. The scientifically sound methods developed by researchers in this project to understand the complex interdependent relationships within integrated systems, as well as their vulnerabilities to threats and hazards, enhance the ability to design more resilient infrastructure solution, identify potential vulnerability in existing systems, and evaluate mitigation strategies.

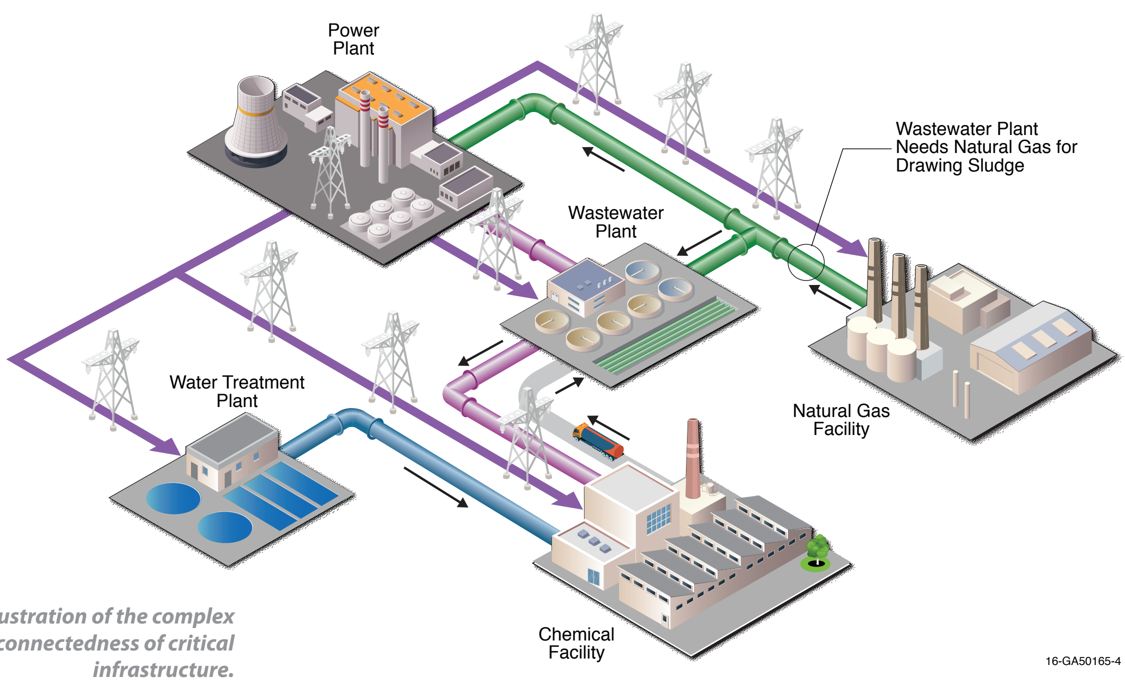


Illustration of the complex interconnectedness of critical infrastructure.

TALENT PIPELINE:

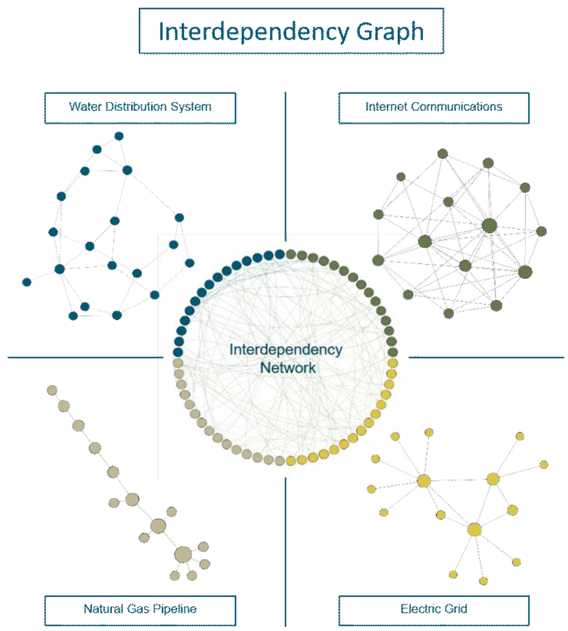
Students:

- Chase Christian, Boise State University
- Christopher Dixon, Indiana University
- Cynthia Lee, Georgia Tech
- Hailey Lynch, Rowan University

PRESENTATIONS:

Dixon, C., R. Hruska, and S. Elliott. 2018. "Dynamics of Multilayer Complex Infrastructure Networks." Presented at the 86th Military Operations Research Society Symposium (Monterey, CA, June 18-21).

Dixon, C., and R. Hruska. 2018. "Dynamics of Multilayer Complex Infrastructure Networks, Dynamics of Multilayer Complex Infrastructure Networks." Presented at Resilience Week. (Denver, CO, Aug. 20-23).



Researchers developed innovative graph representations to capture the maximum dynamics of complex networks.

Detection of Cyber-physical Attack on Nuclear Compliance Monitoring Systems

TOTAL APPROVED AMOUNT:
$125,000 over 1 year

PROJECT NUMBER:
20A1049-005

PRINCIPAL INVESTIGATOR:
Mark Schanfein, INL

CO-INVESTIGATORS:
John Buttles, INL
Hani Mehrpouyan, Boise State University

Researchers designed and prototyped a radio frequency (RF) sensor network that can be deployed within a monitoring cabinet used for nuclear safeguards compliance to detect an attempt to gain access to the inside of the cabinet.

DOE and the International Atomic Energy Agency deploy monitoring cabinets around the world for safeguards compliance. These distributed cabinets are a critical part of the information systems collecting safeguards relevant information on a facility's nuclear material to detect diversion. These cabinets also present a possible cyber physical vulnerability and there is a pressing need to develop technologies capable of quickly identifying and reacting to security events within these systems. Experimentation demonstrated the initial proof of principle of a proprietary RF sensor network designed to go inside the cabinets and detect attempts to gain access. A variety of attack vectors and environmental factors tested the analysis algorithm and led to adjustments to reduce false positives and negatives (i.e., the primary attack vector involved drilling a penetration through the cabinet wall and inserting an Ethernet cable through that penetration at different orientations.) Proof-of-concept of the proposed detection system will be used as the basis for future R&D for applications related to safeguard the monitoring cabinets deployed by the by the DOE and International Atomic Energy Agency for safeguards compliance. This technology improves security for other organizations that keep sensitive equipment in enclosures such as the Departments of Defense, Homeland Security, and State, and commercial entities such as the financial sector and general infrastructure such as power and water.

Example of the type of cabinets deployed by the International Atomic Energy Agency and DOE that will benefit from the RF sensor network monitoring capability.

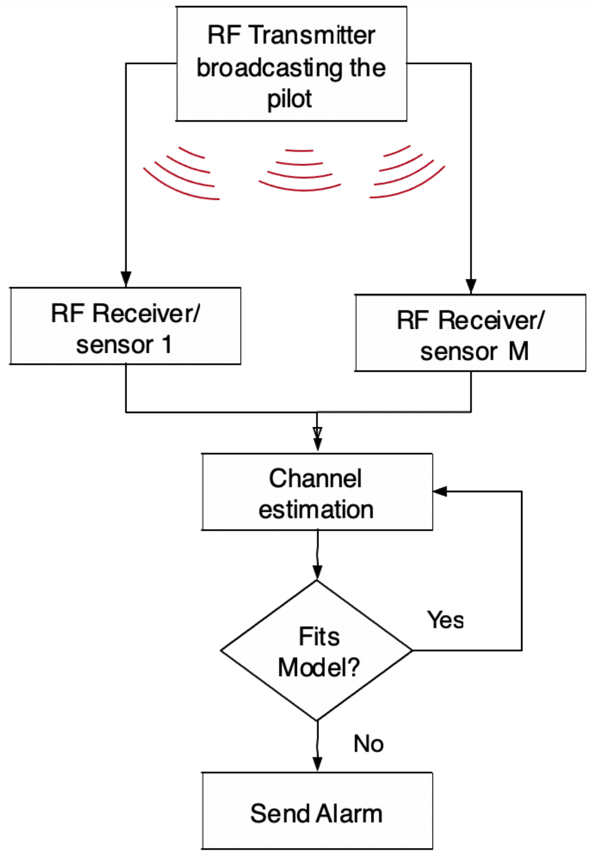
TALENT PIPELINE:

Students:

- Tiffany Bernsten, Boise State University
- Mahfuza Katun, Boise State University

INTELLECTUAL PROPERTY:

One U.S. provisional patent application filed (BA-1227P): Detection of Physical Cyber Attack on High Value Monitoring System Enclosures



System diagram for attack detection with M sensors.

Novel Synthesis of Neptunium Irradiation Targets Through Advanced Electrochemical Techniques

TOTAL APPROVED AMOUNT:
$868,500 over 3 years

PROJECT NUMBER:
18A12-107

PRINCIPAL INVESTIGATOR:
Mathew Snow, INL

CO-INVESTIGATORS:
Edna Cardenas, INL
Chris Dares,
Florida International University
Jared Horkley, INL
Erin May, INL
Jessica Ward, INL

Novel approaches were investigated for producing rare actinide isotopes and converting them into metallic forms as required to support basic nuclear science applications.

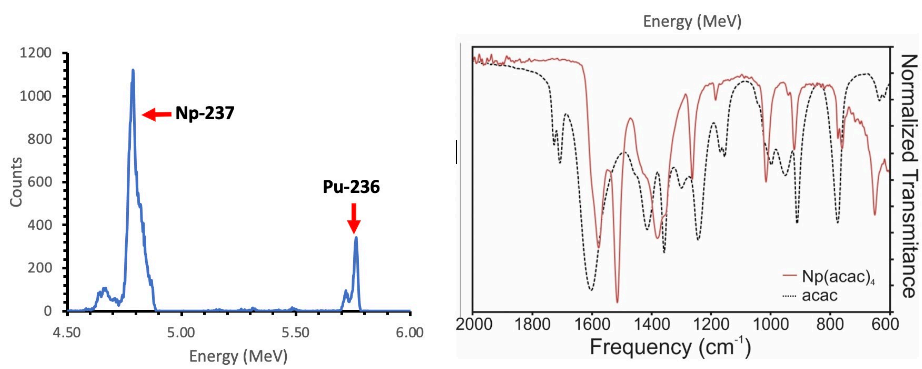
There is a national need for purified actinide isotope materials, including neptunium and plutonium isotopes, to support research in nuclear energy, fundamental nuclear physics, nuclear forensics, and nonproliferation. New methodologies capable of reliably delivering these essential materials are required. This research focused in two primary areas: 1) investigation of novel photonuclear reaction pathways for producing rare actinide isotopes; and 2) exploration of novel solution chemistry synthesis pathways for producing metallic neptunium targets. This resulted in the proof-of-principle for using photonuclear techniques as a future research pathway for production of the rare actinide isotopes neptunium-236m, neptunium-235, and plutonium-236 and the first-ever synthesis of several low-valent inorganic actinide complexes (including neptunium acetylacetonate). This work enables future R&D of macroscopic production of these isotopes for a variety of nuclear science and national security applications, such as advanced nuclear fuels, nuclear safeguards, and nonproliferation.

TALENT PIPELINE:

Students:

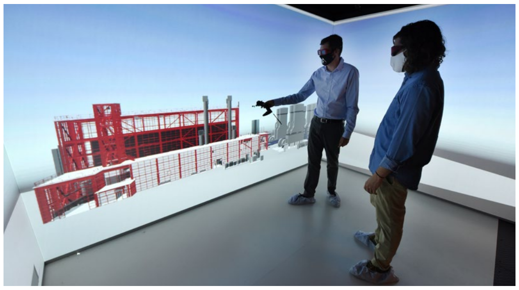
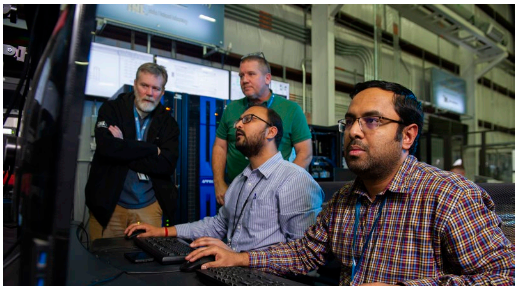
- Creighton King,
  Washington State University
- Jeffery McLachlan,
  Florida International University
- Jessica Ward,
  University of Idaho

INTELLECTUAL PROPERTY:
One U.S. patent (US 10,905,999 B2): Methods for Separating Isotopes from a Sample of Fission Products



Alpha spectra of an irradiated neptunium sample demonstrating photonuclear plutonium-236 production (left) and first-ever fourier-transform infrared spectra of the inorganic neptunium acetylacetonate complex (right).



Idaho National Laboratory

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