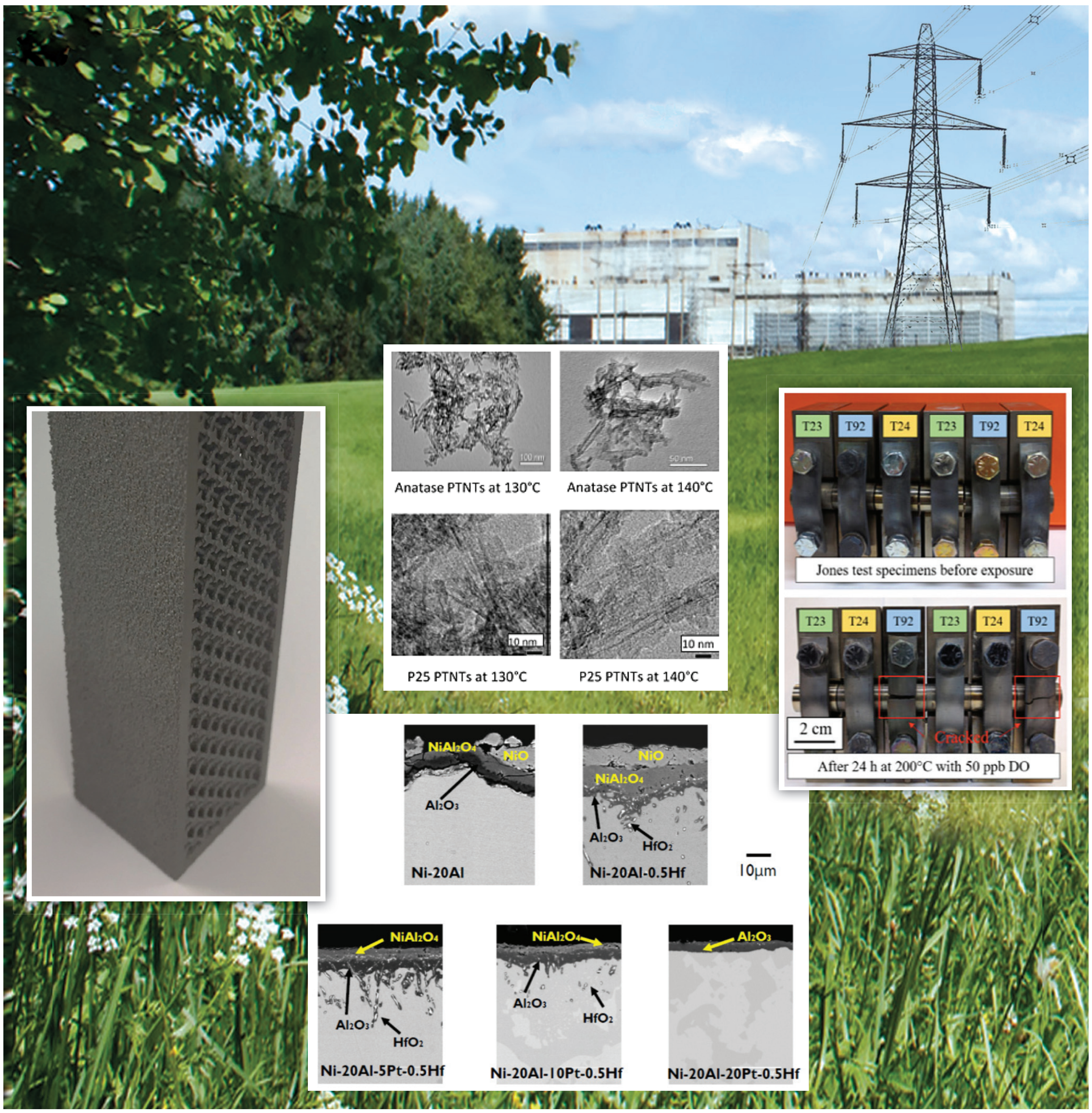
NATIONAL ENERGY TECHNOLOGY LABORATORY

CROSSCUTTING RESEARCH PROGRAM
HIGH PERFORMANCE MATERIALS PROJECT PORTFOLIO



April 2018

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

DISCLAIMER

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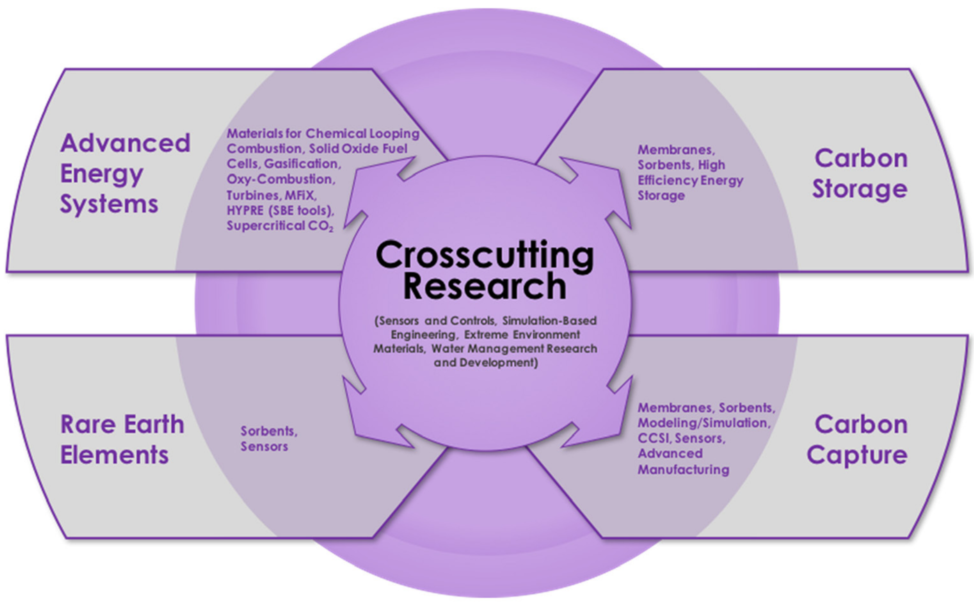
INTRODUCTION

The Crosscutting Research Program develops a range of innovative and enabling technologies that are key to improving existing power systems and essential for accelerating the development of a new generation of highly efficient, environmentally benign fossil fuel-based power systems. The mission space is focused on bridging the gap between fundamental and applied research and development (R&D) efforts. Technologies that successfully bridge this gap are intended to offer viable step-change improvements in power system efficiency, reliability, costs, and environmental impacts.

The research fundamental to the Crosscutting Research Program overlaps and benefits other Office of Fossil Energy (FE) program areas—rare earth elements, carbon capture, carbon storage, and advanced energy systems—as shown in the figure below.



Crosscutting Research technology overlaps with other Fossil Energy Program Areas.

The Crosscutting Research Program executes R&D efforts by partnering and collaborating with research institutions and the power generation industry throughout the United States and in select international locations. The Crosscutting Research Program also sponsors one of the longest running and most important university training and research programs to reinforce the research-based education of students at U.S. universities and colleges with emphasis on fossil energy science. The major objective for this program is to produce tools, techniques, and technologies that map to the Clean Coal Research Program efforts.

The Crosscutting Research Program is comprised of three focus areas: Coal Utilization Sciences, Plant Optimization Technologies, and University Training and Research. A description of each area follows.

Coal Utilization Sciences: The Coal Utilization Sciences technology area research effort is focused on modeling and simulation technologies that lead to a suite of products capable of designing and simulating the operation of next-generation, near-zero-emissions power systems such as gasification and oxy-combustion. Models can also solve current plant operational and lifetime issues. These products are based on validated models and highly detailed representations of equipment and processes.

Plant Optimization Technologies: The Plant Optimization Technologies technology area exists to improve availability, efficiency and environmental performance of coal-based fossil energy power generation plants. Research is focused on sensors and control systems, materials, and water management as the basis for successful implementation of advanced power generation systems in the harsh coal-fired environment. This area also explores novel concepts such as direct power extraction and the application of additive manufacturing towards constructing complex components (e.g., turbine blades with embedded sensing capabilities).

University Training and Research: The University Training and Research (UTR) program awards research-based educational grants to U.S. universities and colleges in areas that benefit the FE and the Crosscutting Research Program. UTR is the umbrella program under which the University Coal Research (UCR) and Historically Black Colleges and Universities (HBCU) and Other Minority Institutions (OMI) initiatives operate. These grant programs address the scientific and technical issues key to achieving Fossil Energy's goals and build our nation's capabilities in energy science and engineering by providing hands-on research experience to future generations of scientists and engineers. The program also coordinates with and seeks opportunities to partner with State and Tribal governments and engage industry, universities, and non-governmental organizations (NGOs) on the responsible use of fossil fuels nationally and internationally.

In addition to the Crosscutting Research Program listed above, the National Energy Technology Laboratory (NETL) uses its participation in the U.S. Department of Energy's (DOE) Office of Science **Small Business Innovation Research (SBIR) Program** to leverage funding, enhance the research portfolio, and, most importantly, facilitate a pathway to commercialization. SBIR is a highly competitive program that encourages small businesses to explore technological potential and provides the incentive to profit from commercialization. By including qualified small businesses in the nation's R&D arena, high-tech innovation is stimulated and the United States gains entrepreneurial spirit to meet specific research and development needs. SBIR targets the entrepreneurial sector because that is where most innovation and innovators thrive. By reserving a specific percentage of Federal R&D funds for small business, SBIR protects small businesses and enables competition on the same level as larger businesses. SBIR funds the critical startup and development stages and encourages the commercialization of the technology, product, or service which, in turn, stimulates the U.S. economy. Since its inception in 1982 as part of the Small Business Innovation Development Act, SBIR has helped thousands of small businesses compete for Federal research and development awards. These contributions have enhanced the nation's defense, protected the environment, advanced health care, and improved our ability to manage information and manipulate data.

The Crosscutting Research Program fosters the development of innovative power systems by conducting research in these key technology areas:

Sensors and Controls: The basis for this research area is to make available new classes of sensors and measurement tools that manage complexity; permit low cost, robust monitoring; and enable real-time optimization of fully integrated, highly efficient power-generation systems. Sensor development focuses on measurements to be made in high temperature, high pressure, and/or corrosive environments of a power system or underground injection system. Harsh environment sensing concepts and approaches focus on low cost, dense distribution of sensors; exploration of sensor networking using passive and active wireless communication; and thermoelectric and vibration energy harvesting approaches. Advanced manufacturing techniques focus on how to lower cost and improve fabrication of sensors. Controls research centers on self-organizing information networks and distributed intelligence for process control and decision making.

High Performance Materials: Materials development under the Crosscutting Research Program focuses on structural materials that will lower the cost and improve the performance of fossil-based power-generation systems and on functional materials, which are designed to perform specified non-structural tasks (e.g., shape memory materials or barrier coatings). Computational tools in predictive performance, failure mechanisms, and molecular design of materials are also being developed to support highly-focused efforts in materials development and reduce the time and cost to develop new materials. Advanced manufacturing development is represented under High Performance Materials in two capacities: first, the need for advancements in feedstocks such as metal powders for superalloys and second, as a set of methods for producing high-performance materials.

Simulation-Based Engineering: This key technology area comprises the expertise and capability to computationally represent the full range of energy science from reactive and multiphase flows up to a full-scale virtual and interactive power plant. Science-based models of the physical phenomena occurring in fossil fuel conversion processes and development of multiscale, multi-physics simulation capabilities are just some of the tools and capabilities in Simulation-Based Engineering. This key technology area enables the development of innovative, advanced energy systems by developing and utilizing advanced process systems, engineering tools and approaches, and the transformation of computationally intensive models into reduced order, fast, user-enabled models for the purposes of study, development, and validation. These tools will be used to optimize data handling and exploit information technology in the design of advanced energy systems with carbon capture.

Water Management Research and Development: Water research encompasses the need to reduce the amount of freshwater used by power plants and to minimize any potential impacts of plant operations on water quality. Research in effluent treatment and water quality sensing, field testing of technologies and processes for treating water produced by injection of carbon dioxide into deep saline aquifers, and exploration of water-limited cooling and innovative multi-stage filtration technologies are being conducted. Data modeling and analysis is being employed to examine existing water availability data on a regional basis. The vision for this program area is to develop a 21st-century America that can count on abundant, sustainable fossil energy and water resources to achieve the flexibility, efficiency, reliability, and environmental quality essential for continued security and economic health. To accomplish this, Crosscutting Research is needed to lead a critical national effort directed at removing barriers to sustainable, efficient water and energy use, developing technology solutions, and enhancing our understanding of the intimate relationship between energy and water resources.

HIGH PERFORMANCE MATERIALS

Power generation plants operate under extreme conditions from a materials standpoint. Future advanced generation facilities will be expected to withstand harsher environments due to higher demands for increased efficiency, quicker plant startups and turndowns, cycling, and alternative power source supplementation. To support these expectations, new materials are needed for these conditions and performance expectations.

Advanced ultrasupercritical (AUSC) boilers, pressurized oxy-combustion boilers, pressurized gasifiers, and the advanced turbines for each of these types of plants will operate under higher temperatures and pressures, which promote rapid corrosion and degradation of subcomponent materials. Internal material stresses in thick-walled components such as superheater headers, turbine casings, and turbine rotors, along with boiler tube scaling and turbine blade erosion, are critical material issues that must be addressed for reliable plant operation.

High-Performance Materials (HPM) focuses on materials that will lower the cost and improve the performance of existing and advanced fossil-based power-generation systems. There are four research areas within HPM:

- Advanced Manufacturing for High Performance Structural and Functional Materials
- Advanced Structural Materials for Harsh Environments
- Computational Based Materials Design & Performance Prediction
- Functional Materials for Process Performance Improvements

Specific Technology Objectives:

- Develop computational materials modeling to enable rapid design and simulation of new and novel alloy materials with reduced repetitive testing. Computational design of materials has the potential to produce major breakthroughs.
- Develop superalloys and ferritic materials for use in AUSC conditions of 760 degrees Celsius (°C) and 350 bar pressure (5,000 psi) to reduce costs, improve corrosion and erosion resistance, increase material strength, and reduce wall thickness.
- Develop functional materials for energy storage and high-performance materials with mechanical properties that can perform reliably at temperatures well over 1,000 ºC.
- Develop advanced metallic and ceramic coatings, including nanomaterials, to provide thermal barrier protection for turbine blades, combustor components, and tubing.
- Validated computational models capable of simulating and predicting performance of materials in various types of transformational power plants, including pressurized oxy-combustion, pressurized gasification, and carbon dioxide (CO_2) cycle plants.

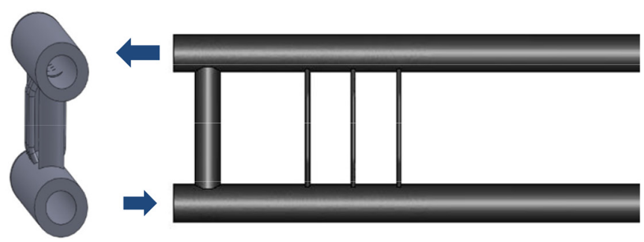
This project portfolio report showcases 39 high-performance materials projects within the Crosscutting Research Program of the Technology Development & Integration Center. Each of the pages reporting on projects clearly describes the technology, the program goals, and overall benefits.

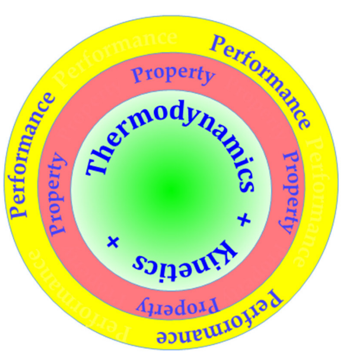
PROJECTS BY RESEARCH AREA

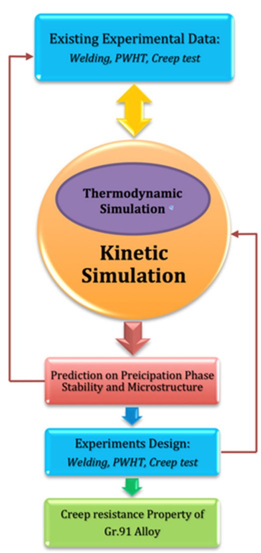
Fuel Injector Tip Model

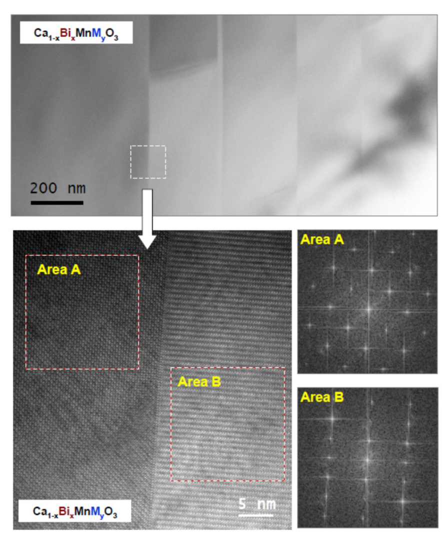
Phenix Printer

Fuel Injector Tip Finished Part



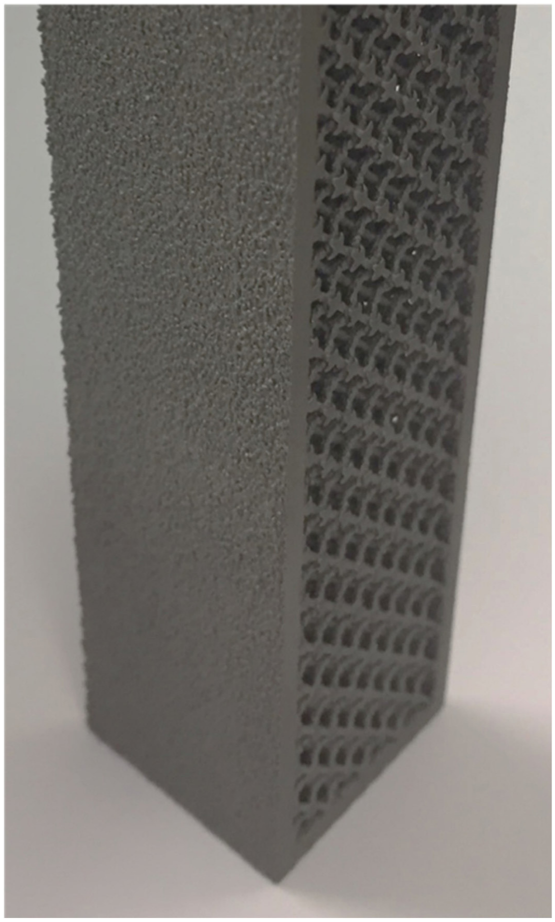






ADVANCED MANUFACTURING

The objective of Advanced Manufacturing for High Performance Structural and Functional Materials is to advance technologies to fabricate, assemble, and join components from high performance materials for advanced fossil energy (FE) power generation technologies.



Example of a complex Haynes 282 mesh structure fabricated by electron beam melting.

PERFORMER(S)	PROJECT TITLE	PAGE
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Oak Ridge National Laboratory	Additive Manufacturing of High Gamma Prime Alloys	13
Oak Ridge National Laboratory	Microstructure and Properties of Ni-based Components Fabricated by Additive Manufacturing	14
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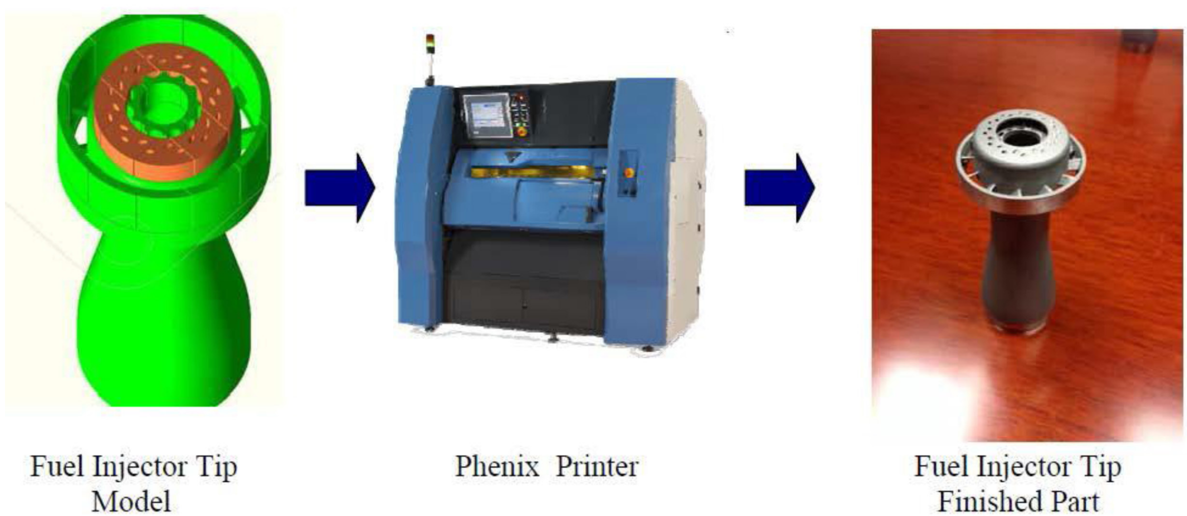
Additive Manufacturing of Fuel Injectors

Performer	Edison Welding Institute, Inc.
Award Number	FE0023974
Project Duration	10/01/2014 – 10/31/2017
Total Project Value	$ 632,447
Collaborator	Solar Turbines Incorporated
Technology Area	Plant Optimization Technologies

NETL is partnering with Edison Welding Institute, Inc. to develop a novel process to qualify the additive manufacturing (AM) technique of laser powder bed fusion for manufacturing complex gas turbine components made of high-temperature nickel-based alloys. Using a fuel injector as a final demonstration piece, project personnel will investigate the effect of input powder stock and AM process variables on resultant microstructure and mechanical properties of the alloy material. Post-processing, including heat treatment and the use of finishing technologies, will also be employed in order to achieve dimensional and surface finish requirements for the component. The benefit will include the development of an AM process that can improve both material and mechanical properties as well as reduce manufacturing cost with little to no impact on durability compared to a traditional investment casting process.

This project will assist in evaluating other turbine components for future AM fabrication. The AM flexibility will allow industrial gas turbine manufacturers to design features into the components that may improve turbine performance and durability. It may also result in lower costs by reducing manufacturing time and eliminating scrap material.



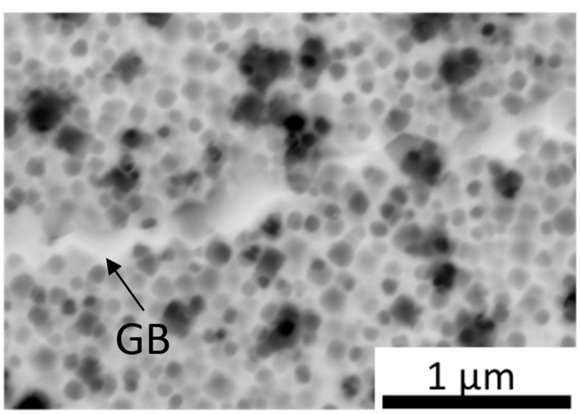
50,000-foot view of AM.

Additive Manufacturing of High Gamma Prime Alloys

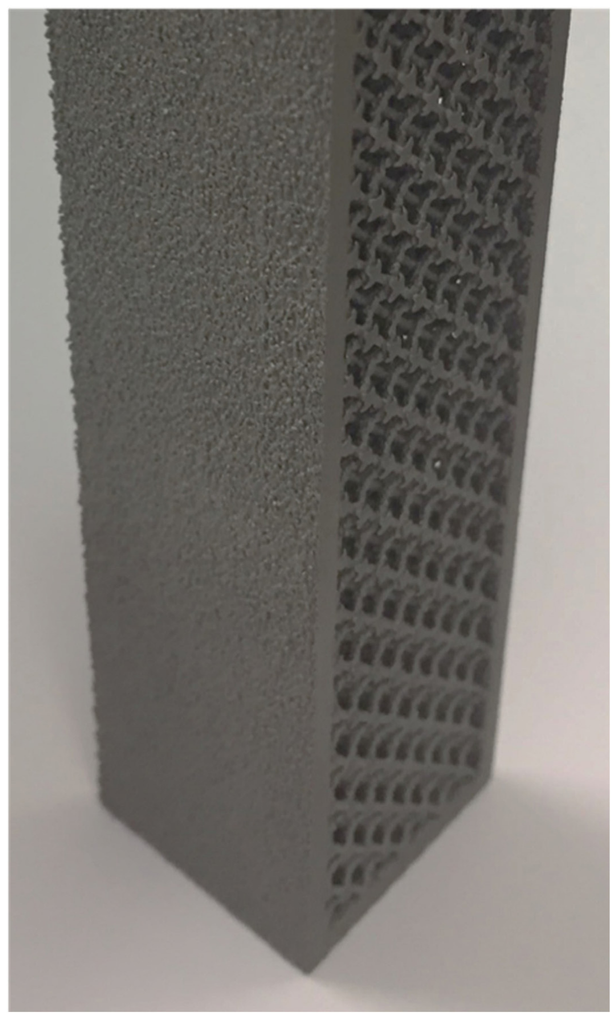
Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA127
Project Duration	09/01/2017 – 09/30/2018
Total Project Value	$ 424,000
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to develop advanced components from high gamma prime alloys (Haynes 282/ Nimonic 105) via innovative manufacturing approaches to enable high temperature/high pressure operation and realize high plant cycle efficiency for advanced ultrasupercritical steam systems (with relevance to gas turbines also). There are several key challenges currently confronting the additive manufacturing (AM) processes for high gamma prime alloys. It is universally recognized that the internal microstructures and performance under load are all dependent on the manufacturing process. Due to the large parameter sets applicable in AM processes and their impact on achievable materials properties and quality, a design of experiments approach will be utilized to achieve the optimal crack-free microstructure with acceptable density.

For AM of high gamma prime alloys, where the understanding of the effects of feedstock properties, deposition rates, thermal history, cooling rates, defect formation and residual stress are still in an early phase, the design of experiments approach will achieve the optimal part properties (density/mechanical properties), surface finish and performance, similar to the rolled plate material. Collaboration between ORNL and Siemens will provide the unique opportunity of developing the process parameters, part microstructure/surface finish, and bulk properties for alloy 282 and Nimonic 105. The final goal is to fabricate Haynes 282 and Nimonic 105 components that are of interest to the AUSC program.



Back scattered scanning electron images of alloy 282 fabricated by electron beam melting showing the grain boundary (GB) carbides and fine gamma prime precipitates in the as-built condition.



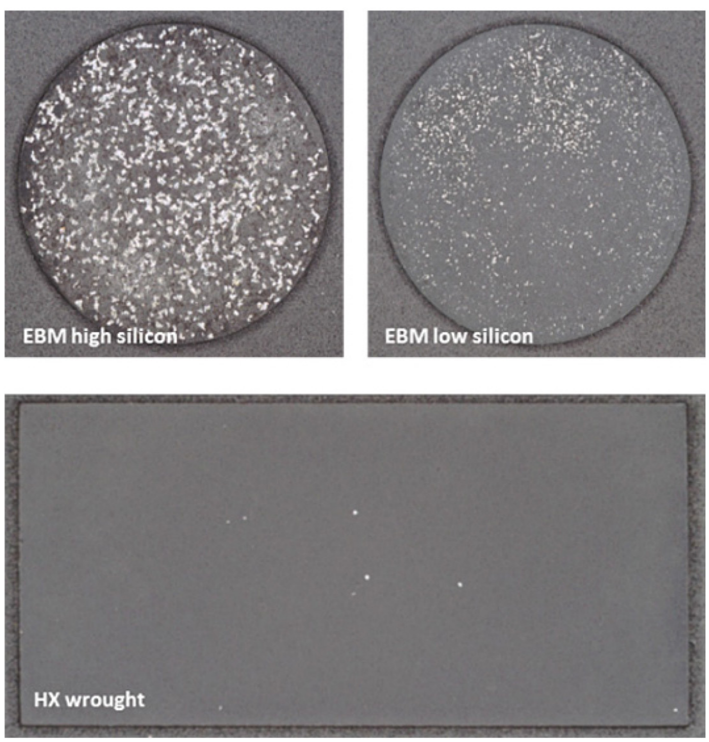
Example of a complex Haynes 282 mesh structure fabricated by electron beam melting.

Microstructure and Properties of Ni-based Components Fabricated by Additive Manufacturing

Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA119
Project Duration	10/01/2015 – 09/30/2018
Total Project Value	$ 954,000
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to optimize the additive manufacturing (AM) fabrication process to produce gas turbine components made of high-temperature nickel (Ni)-based Hastelloy X (HX) alloy. The project team will compare results for HX alloy products made using the three main AM techniques: electron beam melting, laser metal deposition, and selective laser melting. The team will perform extensive microstructure characterization and mechanical testing to determine the relationships among the deposition process, microstructure, and mechanical properties. The mechanical properties of actual gas turbine components fabricated via additive manufacturing will be measured and, as a final step, the three AM processes will undergo cost analyses to determine the potential benefits of using electron beam melting, laser metal deposition, or selective laser melting over conventional fabrication routes.

The technology will be used to produce high-temperature gas turbine components as well as similar-sized components for other advanced fossil energy applications.



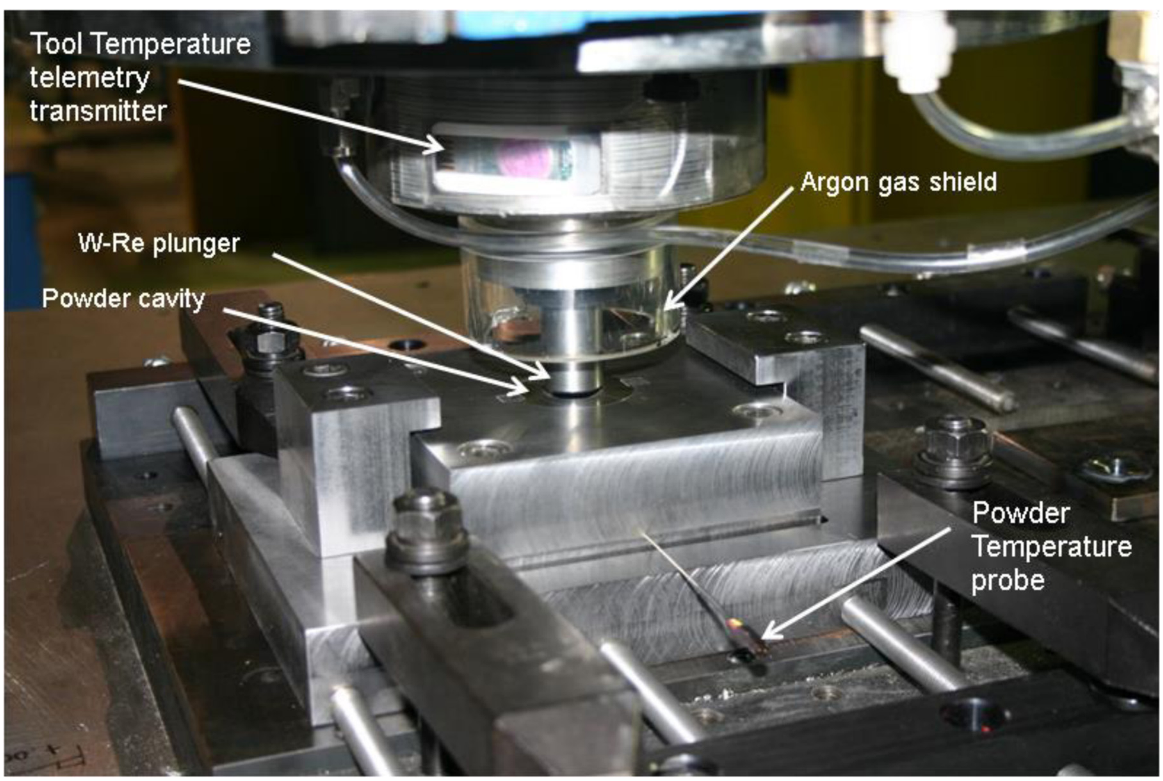
No spallation for wrought HX 4x100 hours at 950 °C.

Low Cost Fabrication of ODS Materials

Performer	Pacific Northwest National Laboratory (PNNL)
Award Number	FWP-60098
Project Duration	10/01/2010 – 09/30/2018
Total Project Value	$ 735,000
Technology Area	Plant Optimization Technologies

NETL is partnering with PNNL to develop a process to fabricate oxide dispersion-strengthened (ODS) materials at lower cost than current manufacturing methods used for these materials, and thus overcome that barrier to their deployment. One approach to enabling the full potential of ferritic ODS materials in an advanced fossil energy power plant cycle is to reduce manufacturing defects and production costs using a new processing methodology. PNNL's recent progress in friction stir welding of ODS alloys suggests that stainless steel powder and oxide powder can be directly mixed and consolidated into full-density rod and tube shapes via a one-step friction stir or shear consolidation process. This project will investigate the new powder metallurgy process, which has the potential to significantly reduce the cost of fabricating ODS products and enable their use in coal and other fossil fuel power plant applications.

The project will contribute to more efficient use of fossil fuels in advanced ultrasupercritical power plants, which will concurrently lead to reduced discharge of carbon dioxide and other emissions.



Friction extrusion die at Pacific Northwest National Laboratory.

Solid State Joining of Creep Enhanced Ferritic Steels

Performer	Pacific Northwest National Laboratory (PNNL)
Award Number	FWP-66059
Project Duration	10/01/2014 – 09/30/2018
Total Project Value	$ 1,075,000
Technology Area	Plant Optimization Technologies

NETL is partnering with PNNL to develop friction stir welding, an alternative solid state joining technology that can enable higher performance from creep strength enhanced ferritic (CSEF) steels anticipated for use in advanced ultrasupercritical (AUSC) coal-fired power plants. A primary problem afflicting welded CSEF steels is that the welds of these steels fail (Type IV cracking) under high temperature at a creep life far below that of the base metal. This problem has led to a reduced performance envelope and either a calculation of reduced strength and lifetime for assemblies made from these alloys, or the use of expensive post-weld heat treatment procedures to recover base metal creep strength in the weldment. Previous work at PNNL on the NETL funded project "Joining of Advanced High-Temperature Materials" (FWP-12461) showed that the friction stir welding process is capable of producing welds in Grade 91M CSEF plate that have significantly improved creep performance over equivalent fusion welds.

It is expected that higher performance CSEF steels used in AUSC coal-fired power plants will improve efficiency and operational flexibility and result in lower operating costs.

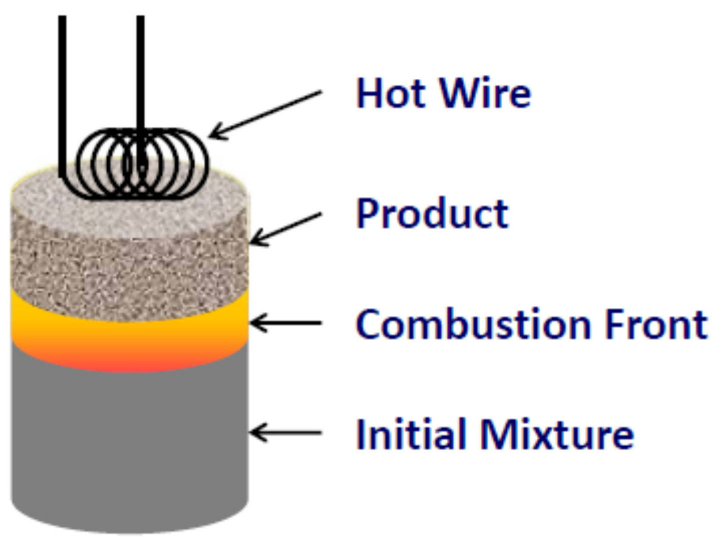
Flat plate friction stir welds in HSLA65 plate.

Combustion Synthesis of Boride-Based Electrode Materials for Magneto Hydrodynamic (MHD) Direct Power Extraction

Performer	University of Texas at El Paso
Award Number	FE0026333
Project Duration	10/01/2015 – 08/31/2019
Total Project Value	$ 250,000
Technology Area	University Training and Research

NETL is partnering with the University of Texas at El Paso to develop a novel technology for advanced low-cost manufacturing of boride-based ultra-high-temperature ceramics for direct power extraction applications. The project will determine optimal conditions of mechanical activation, self-propagating high-temperature synthesis (SHS), and pressureless sintering for fabricating doped zirconium diboride (ZrB_2) and hafnium diboride (HfB_2) that possess all the required properties needed to function as sustainable magnetohydrodynamic electrodes. The project will also determine thermophysical, electrical, mechanical, and oxidation properties of borides obtained by mechanically activated SHS followed by pressureless sintering. This effort will focus on the use of inexpensive materials such as zirconium dioxide (ZrO_2), hafnium dioxide (HfO_2), boron trioxide (B_2O_3), magnesium (Mg), and sodium chloride (NaCl), which could lead to significantly lower production costs compared to synthesis from elements.

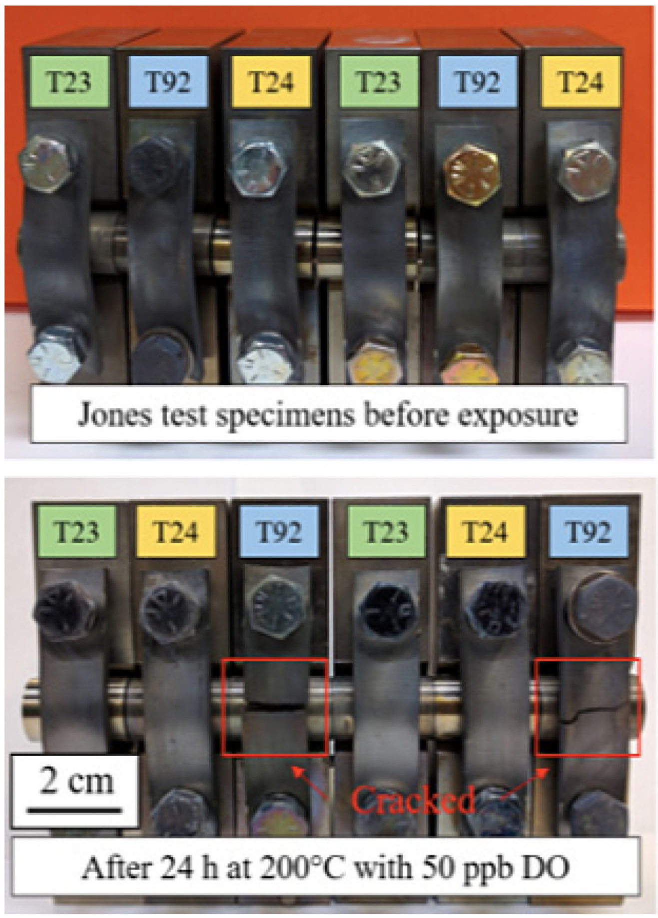
The technology developed in this project will solve certain problems associated with SHS, such as difficult ignition of low-exothermic mixtures and high porosity of products, while exploiting SHS advantages such as low cost, low energy consumption, and high product purity.



Schematic of SHS process.

STRUCTURAL MATERIALS

The objective of the Structural Materials for Harsh Environments subprogram is to develop advanced structural materials that are needed for the harsh operating environments (e.g., high temperature and pressure) of advanced FE power generation technologies.



Jones tests with controlled water chemistry.

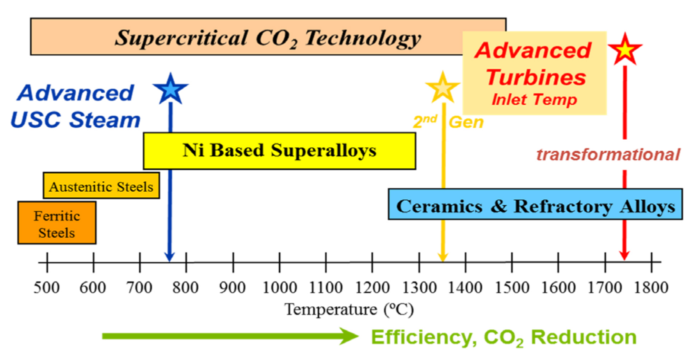
ExtremEMat: Extreme Environment Materials

Performer	Ames National Laboratory	Idaho National Laboratory	Los Alamos National Laboratory	Lawrence Livermore National Laboratory	Oak Ridge National Laboratory	Pacific Northwest National Laboratory
Award Number	FWP-AL-17-510-091	FWP-B000-17016	FWP-FE-850-17-FY17	FWP-FEW0234	FWP-FEAA134	FWP-71133
Project Duration	09/01/2017-09/30/2018	09/01/2017-09/30/2018	09/17/2017-09/30/2018	09/01/2017-09/30/2018	09/01/2017-09/30/2018	09/01/2017-09/30/2018
Total Project Value	$32,000	$150,000	$250,000	$32,000	$150,000	$150,000
Total Value (All)	$764,000					
Technology Area	Coal Utilization Sciences					

The objective of the proposed work is to demonstrate how modern experimental and modeling tools can be integrated across the national laboratory (NL) enterprise with industry partnership to accelerate the development and deployment of new extreme environment materials (EEM) for fossil energy applications. These tools will be developed to accelerate the design and manufacture of a wide range of extreme environment alloys, including Fe-based, Ni-based and high entropy alloys.

Initially, our effort will target enabling supercritical CO_2 (sCO_2) technologies through the development of high yield strength, high-temperature austenitic stainless steel alloys. Although Ni superalloys can meet the performance objectives of sCO_2 technologies, they are costly and may limit the broad application of these technologies. Improvements in the performance of austenitic stainless steels will enable a wider application of these lower cost alloys, thereby reducing the amount and cost of Ni required in the overall system. The challenge is to increase the yield and creep strength of austenitic steels to enable long-term operation at temperatures above 700 °C, while maintaining low cost and manufacturability, using computational tools integrated with experimental characterization. While targeting austenitic alloys, the methodologies developed in this project will be applicable for developing new alloys or for improving the properties and performance of other lower-cost alloys such as 9-12 Cr steels and higher-performance alloys such as Ni-based or high-entropy alloys.

In the near term, the project team hopes to identify promising candidates for new low-cost Fe-based alloys that would perform well in a sCO_2 environment. In the long term, the team hopes to develop and demonstrate a new approach to materials discovery and development for future energy applications. This approach would exploit multiscale (molecular-to-continuum) simulation methods to explore the performance of new materials over wide ranges of compositional space, identifying promising formulations for specific service conditions that can subsequently be tested at the bench scale. This requires demonstrating the ability to overcome major simulation challenges: confidently predicting the properties of metallic alloys over wide ranges of compositional space and the performance life of these materials. If this can be demonstrated, the current laborious approach to materials discovery can be transformed and the path from materials discovery to commercial deployment can be dramatically accelerated. Lastly, the ability to manufacture these new alloys at scale needs to be demonstrated and matured to a level that would encourage industrial adoption in the commercial application.



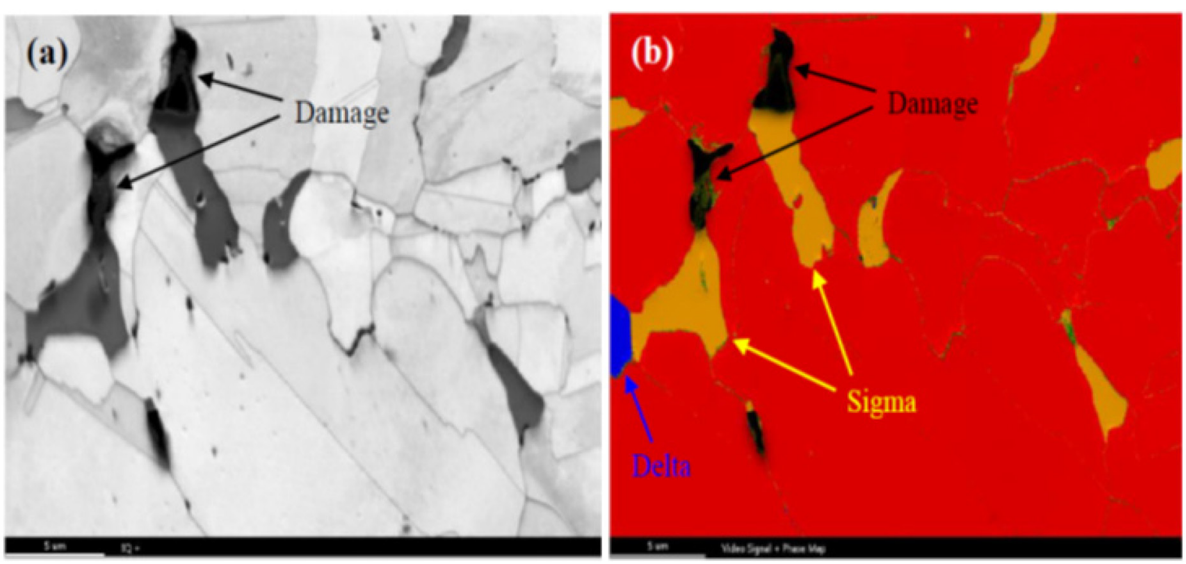
Extreme environment materials for advanced fossil energy power generation.

Characterization of Long-Term Service Coal Combustion Power Plant Extreme Environment Materials (EEMs)

Performer	Electric Power Research Institute, Inc.
Award Number	FE0031562
Project Duration	01/25/2018 – 01/24/2021
Total Project Value	$ 2,500,000
Technology Area	Plant Optimization Technologies

NETL is partnering with the Electric Power Research Institute to provide a comprehensive database of mechanical properties, damage assessment/accumulation, and microstructural information from extreme environment material (EEM) components subjected to long-term service with the intent to develop, calibrate, refine, and/or validate the life assessment tools used for predicting remaining life under complex operating conditions. Sufficient quantities of EEM components will be obtained from operating and decommissioned coal-fired power plants. The materials obtained will have been exposed to long-term service (greater than 100,000 hours) and will include all relevant background information for material type, fabrication data, and operational conditions. The acquired materials will be subjected to detailed damage analysis, in-depth microstructural characterization, and, where relevant, rigorous low- and/or high-temperature mechanical testing in an effort to establish a link between microstructural/damage evolution and long-term behavior as established by in-service performance, destructive evaluation, or predicted behavior through time-temperature-parameter relationships or continuum damage mechanics.

The results obtained from this project will provide a comprehensive compendium of materials data and time-temperature-parameter relationships for EEM components exposed to long-term service in coal-fired power plants.



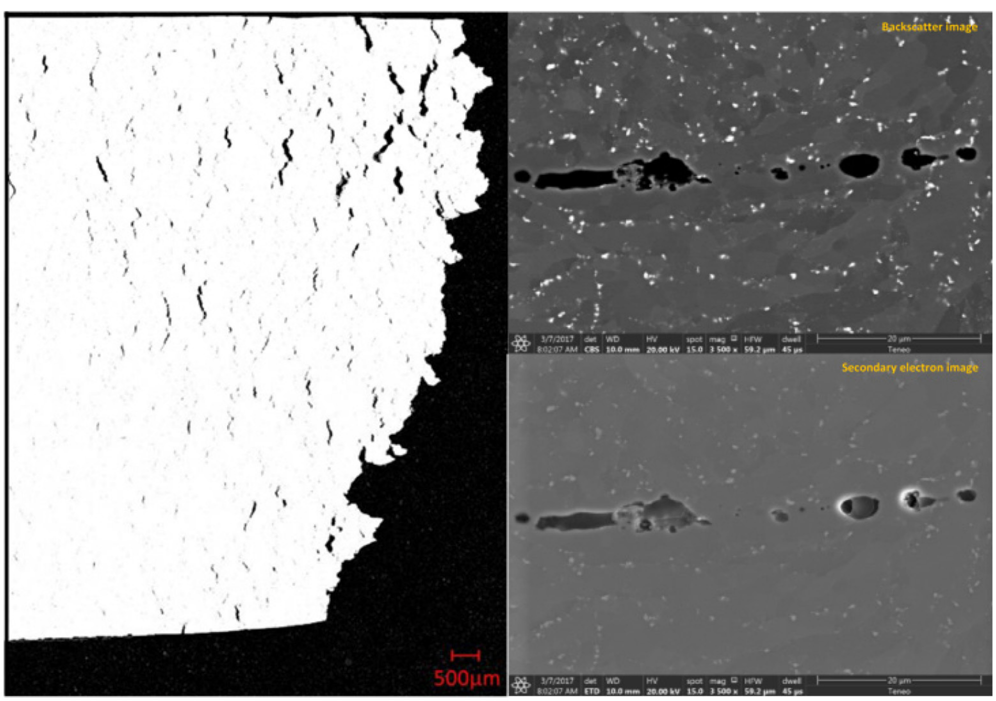
(a) Scanning electron microscope image and (b) corresponding electron backscatter diffraction phase map showing creep damage associated with sigma phase in 374H.

Optimization of Advanced Steels for Cyclic Operation Through an Integration of Material Testing, Modeling and Novel Component Test Validation

Performer	Electric Power Research Institute, Inc.
Award Number	FE0026260
Project Duration	09/01/2015 – 03/31/2018
Total Project Value	$ 786,322
Collaborators	Structural Integrity Associated, Inc. and Wyman-Gordon
Technology Area	Plant Optimization Technologies

NETL is partnering with the Electric Power Research Institute to qualify improved high-performance structural materials for application in current power plants in order to improve operational flexibility. The project will (1) develop the needed microstructural processing and performance relationships and associated material models for specific constituents in fabricated weldments (such as the parent material, heat affected zone regions, and weld metal); (2) apply these metallurgical relationships through modeling to a composite welded component subjected to cyclic operational conditions under both mechanical and thermal loading; and (3) validate the model through novel structural feature and component tests. The project will significantly impact the technical community by improving existing mainstay creep strength enhanced ferritic steels operating under flexible operation modes.

The expected benefits of the project will be lab-scale demonstration of an improved version of P92 and its weldments for use in cycling fossil energy power plants, and a new procedure for testing creep-fatigue and thermo-mechanical fatigue of weldments that bridge the gap between current small specimen lab testing procedures and testing of full-scale power plant components.



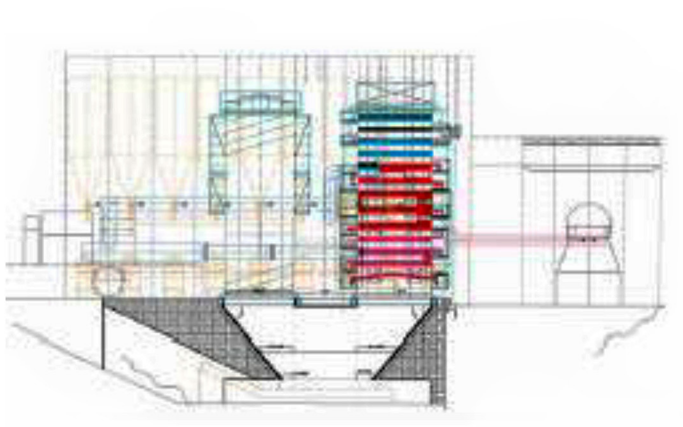
Scanning electron microscopy evaluation of longest duration sample.

Advanced Ultra-Supercritical Component Testing

Performer	Energy Industries of Ohio, Inc.
Award Number	FE0025064
Project Duration	11/01/2015 – 09/30/2021
Total Project Value	$ 74,058,187
Collaborators	AECOM; Electric Power Research Institute, Inc.; GE Power and Water; The Babcock & Wilcox Company; Thermal Engineering; and Youngstown Thermal
Technology Area	Plant Optimization Technologies

NETL is partnering with Energy Industries of Ohio Inc. to demonstrate advanced ultrasupercritical (AUSC) technology at a commercial-scale level of technology readiness by designing, procuring, constructing, and operating a test facility consisting of a prototype R&D-scale (approximately 134,000 lbs./hr. steam flowrate equivalent to 20 MW power generation) AUSC steam turbine and other AUSC plant components needed to generate the steam to run the prototype-scale steam turbine. Project personnel will complete planning activities and front-end engineering design for conducting full-scale pilot testing of select components at high temperatures and pressures.

The expected benefits of the project will be the development of a domestic supply chain for fabricating nickel superalloy and other AUSC power plant components; validation through design, fabrication and operation of a prototype (20 MW) scale unit that an AUSC steam turbine can be designed, built, and reliably operated under both steady-state and varying load operating conditions; development and validation of fabrication, installation, and repair methods for nickel superalloy and other AUSC power plant components; and procurement of sufficient R&D test and metallurgical analysis data to design an AUSC demonstration plant with a high probability of technical success.



Downdraft inverted tower AUSC steam generator.

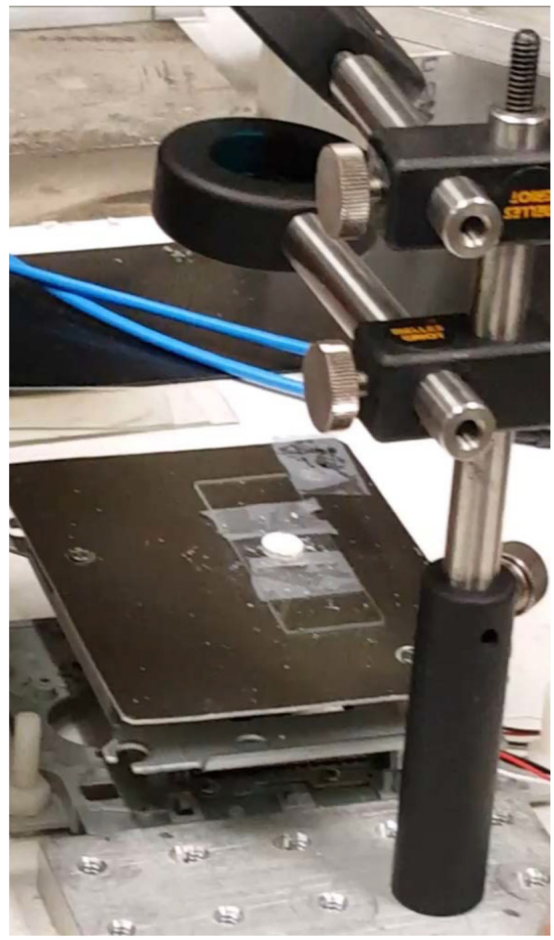
AUSC ComTest superheater arrangement.

Novel High Temperature Carbide and Boride Ceramics for Direct Power Extraction Electrode Applications

Performer	Florida International University
Award Number	FE0026325
Project Duration	10/01/2015 – 09/30/2018
Total Project Value	$ 249,970
Technology Area	University Training and Research

NETL is partnering with Florida International University to develop nano-carbide and -boride ceramic solid solution and related composites via novel synthesis and processing and to understand the fundamental composition-processing-structure-property relationships for materials such as potential hot electrodes for direct powder extraction, e.g., magnetohydrodynamic (MHD) systems. Basic research on new high-temperature ceramic materials, including novel means of synthesis and processing, will be performed. Fundamental knowledge will be developed and leveraged to design direct power extraction applications for cleaner and more efficient power generation using fossil fuels.

This research will provide insights into how fundamental composition-processing-structure-property relationships will support development of these materials for a broad range of applications from energy to aerospace. This research could also significantly impact the development of high- temperature MHD electrodes as well as the fields of advanced ceramics and high-temperature materials science, and could lead to dramatic reductions in the time and energy input during the materials sintering process, resulting in less costly high-temperature ceramic materials.



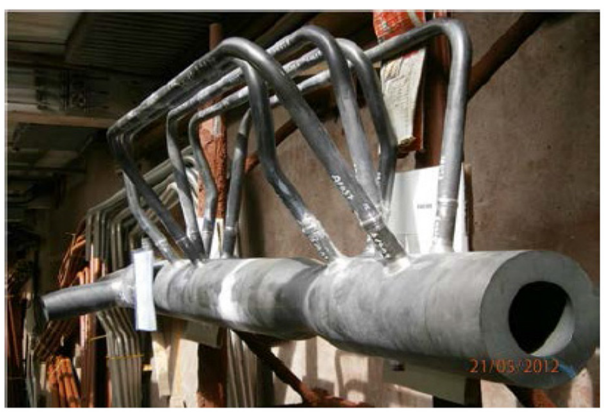
Green body formation via laser cutting.

Advanced Ultrasupercritical (AUSC) Materials Thick-Walled Cycling Header Development for ComTest-AUSC

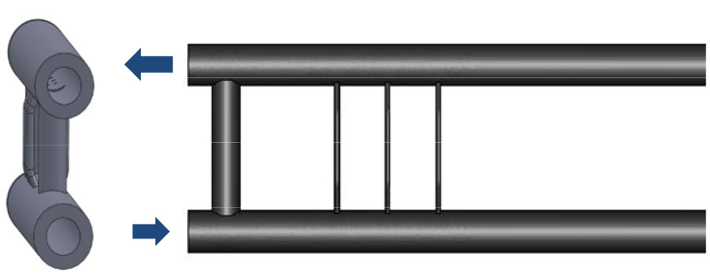
Performer	GE Power (Alstom Power, Inc. prior to the merger of Alstom Power and GE)
Award Number	FE0026183
Project Duration	09/16/2015 – 12/31/2017
Total Project Value	$ 870,520
Technology Area	Plant Optimization Technologies

NETL is partnering with GE Power, Steam Power Systems to develop a design for testing a high- temperature nickel-based superalloy thick-walled header for cycling and flexible plant operation in new advanced ultrasupercritical (AUSC) and existing ultrasupercritical and supercritical plants. This project focuses on developing a design for the high-temperature nickel (Ni)-based superalloy header component typical of a thick-walled header subjected to thermal and pressure cycling of full-scale AUSC steam cycle loading conditions. This upfront analytical simulation of the design will eliminate or minimize potential operational problems for the actual ComTest-AUSC and will lead to successful testing of advanced materials for thick-walled pressure parts such as the headers and piping.

This project will design the layout for the piping system and identify specific instrumentation needed for component testing of the AUSC steam temperature cycling and data logging system required during operation. The project will demonstrate recently developed Ni-based superalloys that can operate at higher temperatures and support future transformational power technologies such as AUSC oxy-combustion, supercritical CO_2 cycles, nuclear power, solar power, and natural gas combined cycle units.



European ComTest header configuration, CCA 617 alloy.



US ComTest AUSC thick-walled cycling header configuration.

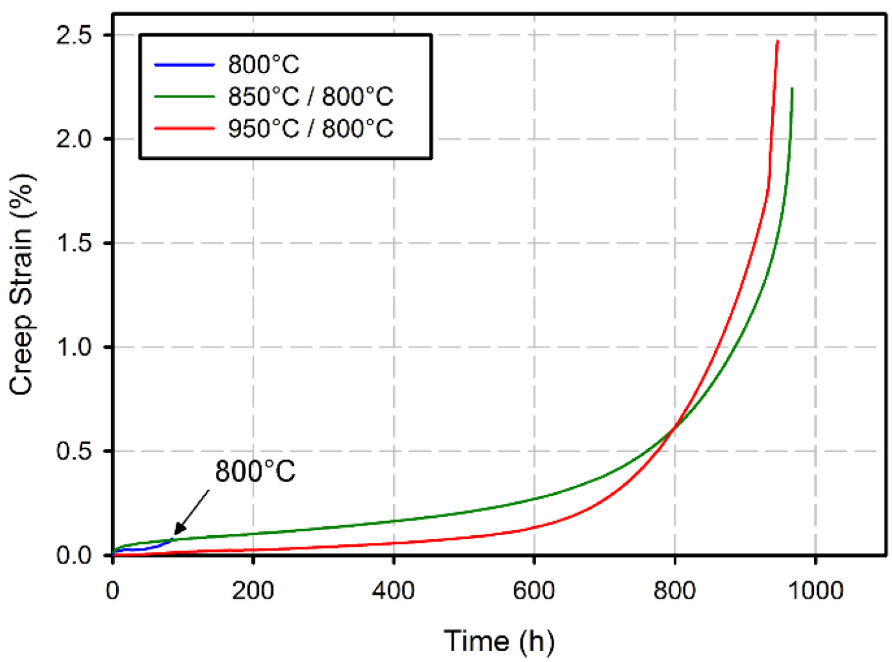
Advanced Alloy Development

Performer	National Energy Technology Laboratory
Award Number	FWP-1022406
Project Duration	01/01/2017 – 03/31/2018
Total Project Value	$ 2,790,000
Technology Area	Plant Optimization Technologies

The Advanced Alloy Development Field Work Proposal (FWP) is focused on developing improved steels, superalloys, and other advanced alloys using an integrated materials engineering approach that incorporates computational alloy design with best practice manufacturing (modified as needed to achieve microstructure and performance objectives) using focused mechanical testing and characterization. Work will also be conducted to develop and validate computational algorithms for designing advanced alloys and for predicting alloy performance over multiple length scales and multiple time scales relevant to advanced fossil energy power systems.

The Advanced Alloy Development FWP has five distinct research themes, three broad in nature with the other two being focused on enabling supercritical carbon dioxide (sCO_2) power plant technology:

- *Systems Engineering & Analysis (SE&A)* – Provide techno-economic and market studies on fossil fuel power generation plants operating at the elevated conditions (e.g., advanced ultrasupercritical (AUSC) Rankine cycles) enabled by advanced alloys, identifying applications and quantifying the cost and performance improvements relative to the commercial state-of-the-art.



Creep curves of a IN740H casting having received different aging treatments.

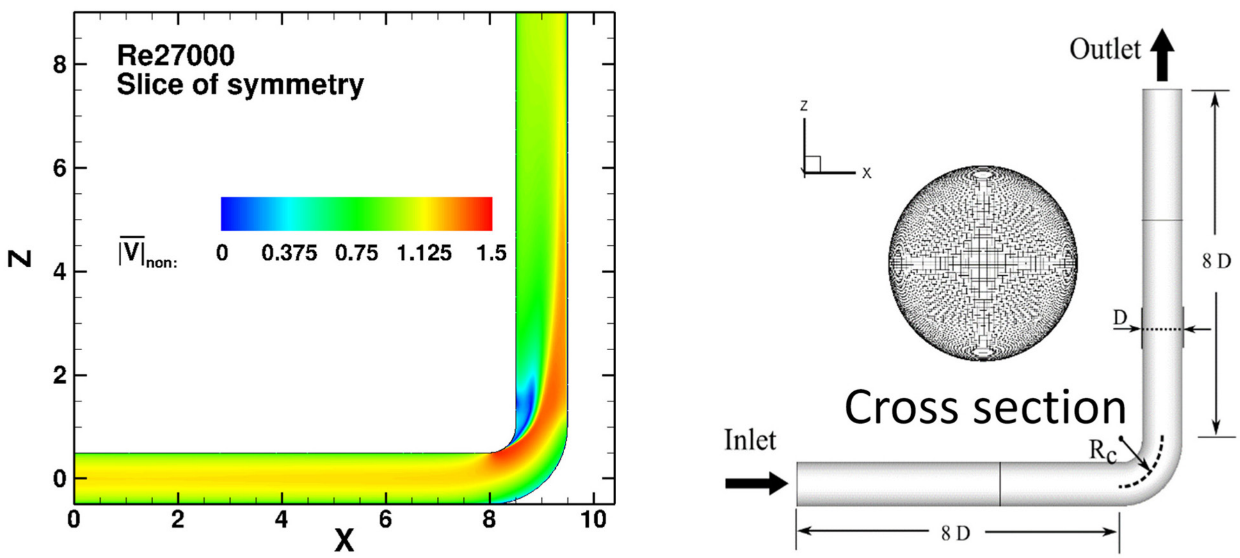
- *Computational Design and Simulation* – Use computational materials modes, multi-scale characterization simulations of microstructural features, and cutting-edge data analytics to guide and accelerate alloy design and manufacturing development.

- *Processes, Manufacturing, and Properties* – Develop and demonstrate at pilot industrial scales improved manufacturing processes to produce advanced alloys with improved service life performance.

- *Materials for sCO_2 Power Cycles: Alloy Performance* – Determine whether available AUSC power plant materials are suitable for fossil fuel sCO_2 service in terms of temperature and stress, and if they are, assess the potential physical and mechanical consequences of their use.

- *Materials for sCO_2 Power Cycles: Materials and Manufacturing Issues Associated with Heat Exchangers for sCO_2 Power Cycles* – Assess materials selection and joining processes for compact heat exchanger designs to (1) reduce equipment size, and (2) enhance heat transfer between the high-temperature and low-temperature working fluids in sCO_2 power cycles.

The structural materials and manufacturing processes researched in this FWP are needed to lower the cost and improve the performance of fossil-based power-generation. Additionally, the development and utilization of computational simulation and broad-based data analytic tools can further reduce the time and cost of developing advanced energy systems.



Large-eddy simulation is implemented using a highly validated, efficient and predictive solver, which is fully parallel and uses finite volume method. Geometry and cross section of the pipe used in simulation is shown on the left. Time averaged velocity along the pipe on the center slice showing faster flows outside after the bend.

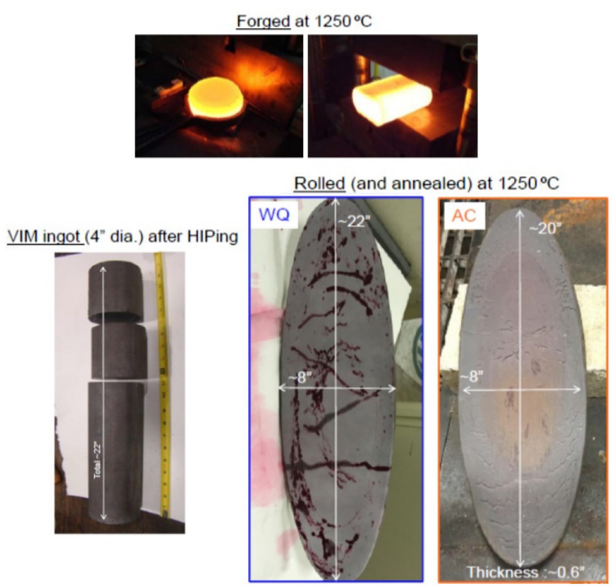
Advanced Alloy Design Concepts for High Temperature Fossil Energy Applications

Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA114
Project Duration	10/01/2013 – 09/30/2018
Total Project Value	$ 1,934,000
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to identify and apply breakthrough alloy design concepts and strategies for incorporating improved creep strength, environmental resistance, and weldability into the classes of alloys intended for use as heat exchanger tubes in fossil-fueled power generation systems at higher temperatures than are possible with currently available alloys.

This work will develop stable microstructures with dispersion of strengthening second-phase precipitates based on guidance from computational thermodynamics and modeling of inter-diffusion, including new directions suggested by ongoing modeling studies in other Crosscutting Research projects; apply mechanistic understanding of the development and evolution of microstructures associated with strengthening phases, and of the influences of and interactions with the concentration and distribution of specific elements necessary to form an inherently-protective outer oxide layer; and use advanced analytical techniques, and especially their evolution as a function of time, temperature, and external environment.

Higher performance from alloys used in fossil-fueled power generation systems at higher temperatures will lead to improvements in efficiency and operational flexibility and result in lower operating costs.



Scale-up efforts (Fe-30Cr-3Al-2Nb-0.2Si-0.12Y).

Advanced Materials Issues in Supercritical Carbon Dioxide

Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA123
Project Duration	10/01/2015 – 09/30/2018
Total Project Value	$ 650,000
Technology Area	Advanced Turbines

This project continues to address the materials issues associated with scaling-up supercritical carbon dioxide (sCO_2) Brayton cycle systems to higher temperatures for increased efficiency and larger size for commercial power production. The effort is intended to understand the applicable corrosion mechanisms in sCO_2 as a function of impurity (e.g., O_2, H_2O) levels in both closed and open systems. Once this experimental capability is established, the experimental plan will also continue to study environmental effects on alloy mechanical properties with complementary efforts in characterization and lifetime modeling.

Alloy-specific temperature limits developed previously and further evaluated in this project will facilitate materials selection and guide initial efforts in alloy design with a goal of lowering the material costs for new utility-size sCO_2 systems.

Specimen coupon holder being loaded into ORNL high-pressure autoclave for testing in supercritical carbon dioxide at 750 °C/300 bar.

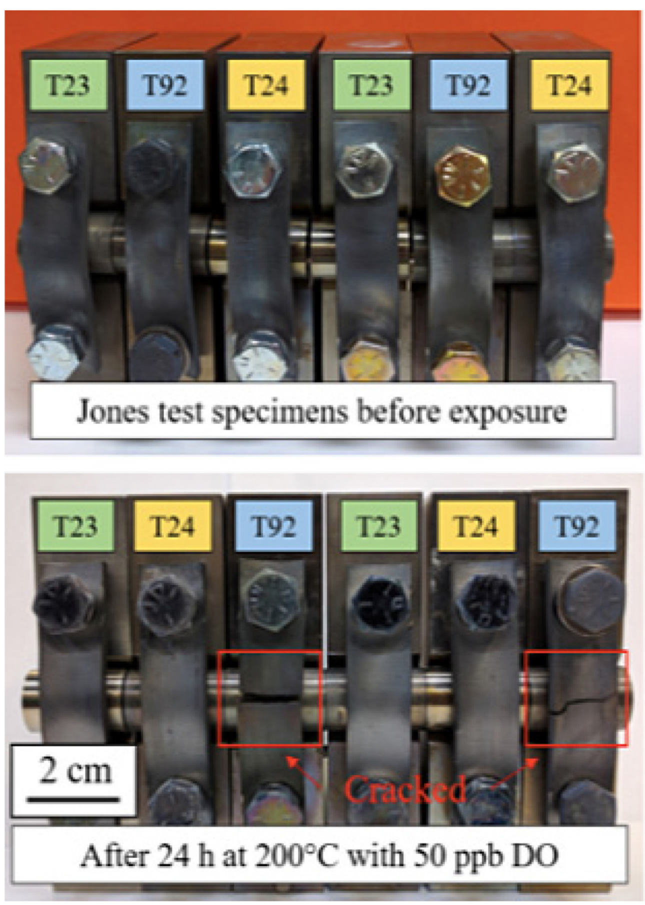
Corrosion Issues in Advanced Coal Fired Boilers

Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA116
Project Duration	10/01/2013 – 09/30/2018
Total Project Value	$ 1,764,250
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to address critical corrosion and environmental effects issues in coal-fired boilers ranging from boiler water walls to superheater tubes. Specific technical objectives are to get a better understanding of (1) hydrogen induced cracking in boiler water walls and which alloys may be more resistant to this type of degradation and (2) the effect of shot peening on steamside oxidation of austenitic superheater tubes. Such knowledge is critical to efforts to develop more accurate lifetime prediction models for current alloys used in boilers, and advanced alloys and surface modifications that are being considered for use in advanced coal-fired power systems.

The project goal will be achieved by determining the temperature-relevant corrosion mechanisms; determining the role of environment on mechanical response; evaluating the upper temperature limit for new materials and surface modifications in terms of lifetime; and characterizing the reaction products and extent of alloy degradation under these conditions.

The results should improve performance of commercial and model alloys in controlled laboratory experiments to simulate advanced fossil boiler conditions.



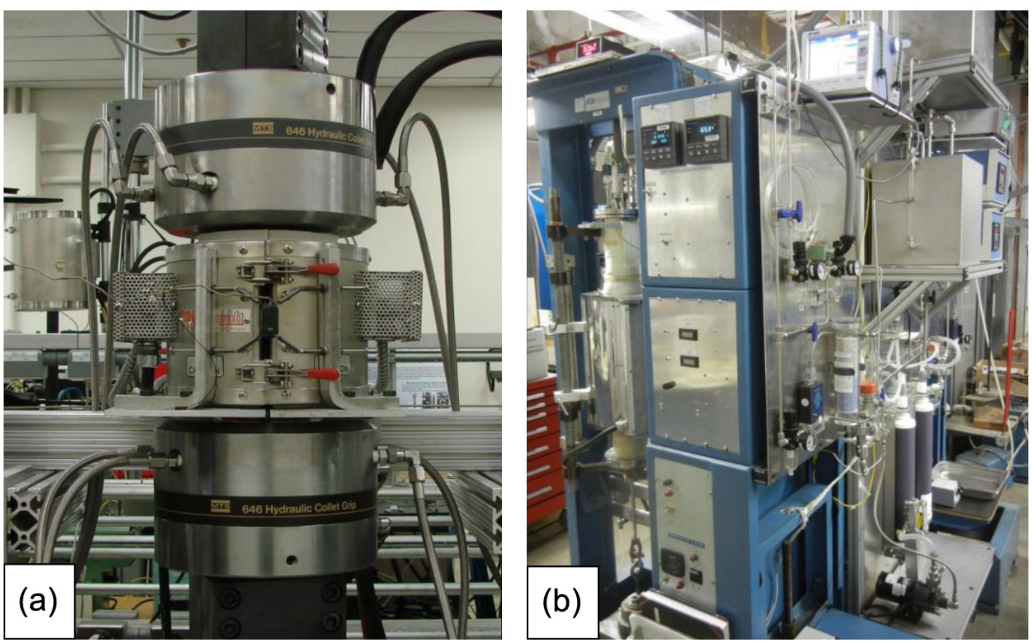
Jones tests with controlled water chemistry.

Creep-Fatigue-Oxidation Interactions: Predicting Alloy Lifetimes Under Fossil Energy Service Conditions

Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA115
Project Duration	10/01/2013 – 09/30/2018
Total Project Value	$ 1,500,000
Technology Area	Coal Utilization Sciences

NETL is partnering with ORNL to generate pertinent creep-fatigue data and develop new lifetime models to help accurately predict the lifetimes of fossil fuel power plant components that are subjected to flexible operation (e.g., load cycle following of renewable power generation). Such flexible operation can cause thermal-mechanical fatigue of components over long periods resulting in their premature failure. Most existing coal-fired power plants were not designed for this type of operation, and new advanced fossil fuel plants may need to include flexible operation in their thermal/mechanical design.

Improvements to creep-fatigue data and lifetime models will advance the development of advanced power plant designs, improve efficiency and operational flexibility, and reduce operating costs.



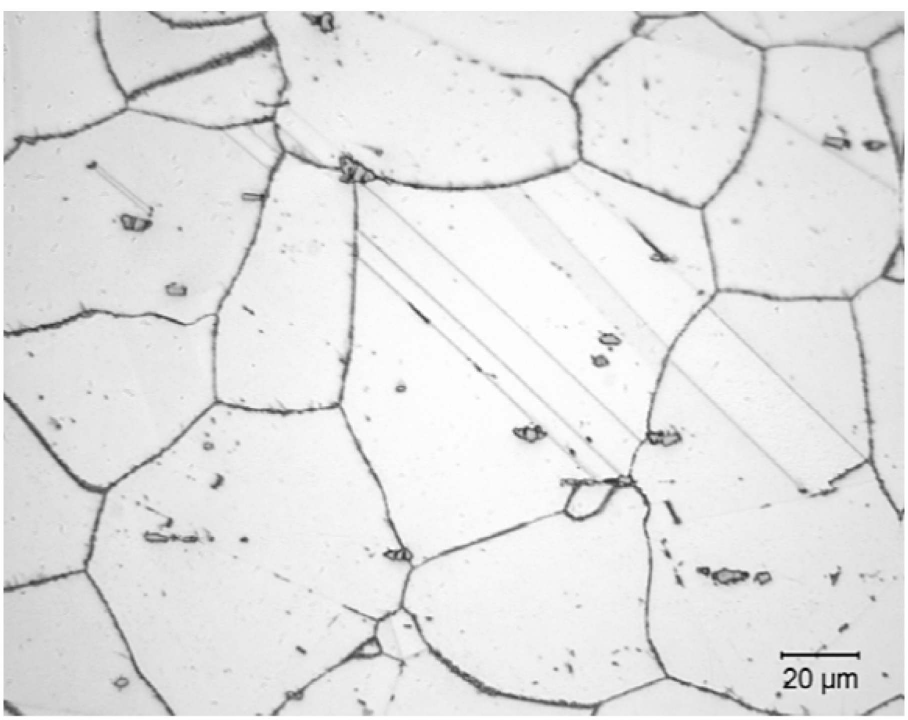
Servo-hydraulic creep-fatigue machine (left) and thermal cyclic creep machines (right) allowing testing in steam.

Materials Qualification and Deployment for High Efficiency Coal Fired Boilers

Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA117
Project Duration	04/01/2015 – 09/30/2018
Total Project Value	$ 820,000
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to address materials issues relevant to qualifying and deploying a nickel (Ni)-based alloy for a new application in an advanced ultrasupercritical coal-fired boiler. The project will deploy Haynes 282 (H282) alloy for application in superheaters, reheaters, and steam delivery pipes by completing base metal and cross-weld creep and tensile testing needed for an American Society of Mechanical Engineers (ASME) Boiler and Pressure Vessel Code Case and the associated microstructural analyses needed for assurance of boiler-relevant lifetimes. Lab work will focus on tensile and creep testing of the base metal and cross welds in the 1,100 to 1,700 °F temperature range.

The goal of this project is to generate the laboratory mechanical properties data needed to obtain ASME Code qualification of single aged H282 nickel superalloy for use in pressure-bearing components of coal-fired boilers and other high-temperature power generation equipment. Microstructural characterization will provide insights into failure mechanisms that will help support extrapolation methods of the lab creep test data to estimated creep strength at 100,000 hr. life.



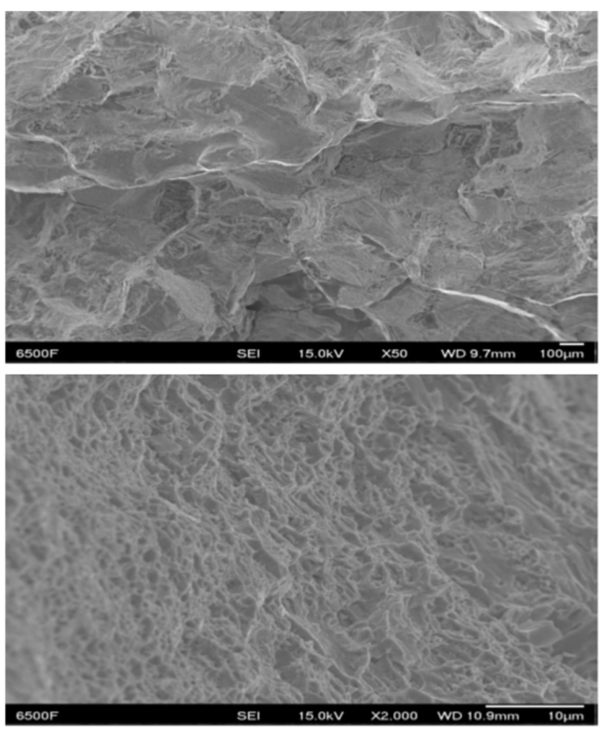
H282 microstructure in age hardened condition.

Properties of Advanced Ni-Based Alloys for A-USC Steam Turbines

Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA125
Project Duration	02/01/2016 – 09/30/2018
Total Project Value	$ 2,160,000
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to evaluate the behavior of high-temperature materials to complement the efforts of the Advanced Ultrasupercritical (AUSC) Steam Turbine Materials Consortium in qualifying alloys for steam turbine designs required for operation under AUSC steam conditions of 760 degrees Celsius (°C) and 345 bar/1400 degrees Fahrenheit (°F) and 5000 pounds per square inch (psig) steam, and in ensuring that any limitations of current materials are overcome. This project will perform creep-testing and microstructural characterization of a large cast valve body of Haynes 282 alloy; evaluate long-term creep resistance of a large forging of Haynes 282 alloy, including the effects of fine grain size; evaluate steam effects and pre-test microcracks on the fatigue behavior of the large forging of Haynes 282 alloy; perform microstructural characterization and longer-term creep testing for dissimilar metal welds of Inconel 740H pipe joined to Haynes 282 alloy valve casting; develop constitutive equations or predictive models and upgrade the damage evaluation and life-prediction criteria; and perform tests to assess the effects of CO_2 on mechanical behavior.

This project will reduce the quantity and cost of components made from nickel superalloys by developing more precise mechanical behavior data that can be used to produce more accurate models of the mechanical behavior of these components under varying high temperature and applied stress conditions.



Cast Haynes 282 fractures mainly along heavily precipitated dendrite colony boundaries.

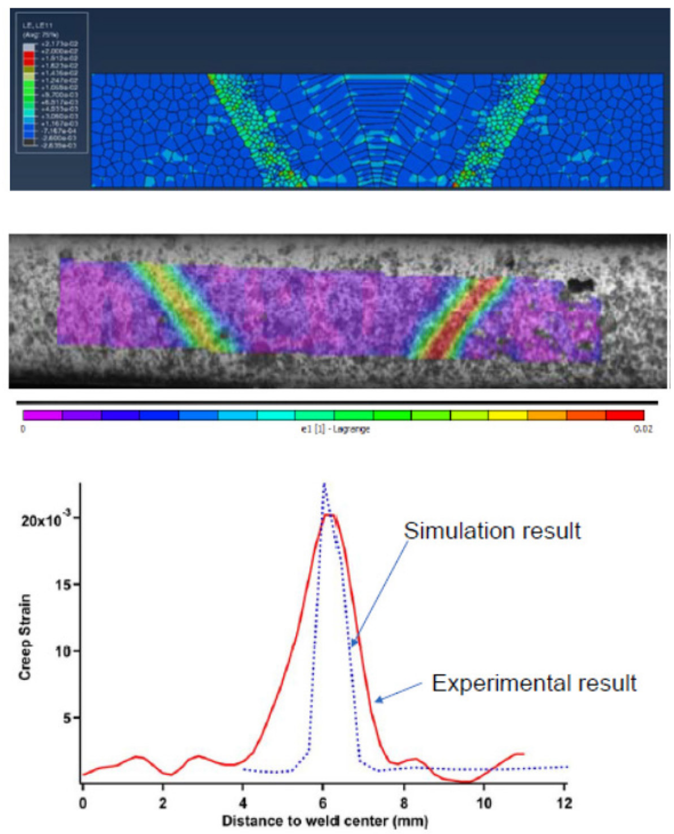
Weldability of Creep Resistant Alloys for Advanced Power Plants

Performer	Oak Ridge National Laboratory (ORNL)
Award Number	FWP-FEAA118
Project Duration	10/01/2013 – 09/30/2018
Total Project Value	$ 1,450,000
Technology Area	Coal Utilization Sciences

NETL is partnering with ORNL to develop practical engineering solutions to two key issues regarding the weldability of high-temperature creep-resistant alloys used in advanced fossil energy power plants: (1) the reduced creep strength of the weld region vs. the base metal and (2) welding of dissimilar metals.

The work will develop fundamental mechanistic understanding of the weld failure process using advanced in-situ neutron and synchrotron experimental techniques and a state-of-the-art integrated computational welding mechanics modeling tool (ICWE) developed at ORNL; apply the ICWE modeling tool to simulate the microstructure and property variations in the weld region; develop an improved weld creep testing technique using digital image correlation to accurately measure the localized non-uniform deformation of a weld under high-temperature creep testing conditions; determine the local creep and creep-fatigue constitutive behavior in different regions of a weld; and develop new welding and post heat treatment practices to improve the creep resistance of similar and dissimilar metal weldments.

The research will promote the design of advanced power plants capable of operating at higher temperatures and pressures, thus improving their efficiency and operational flexibility and reducing capital and operating costs.



Top: Modeling result.

Middle: Experimental result.

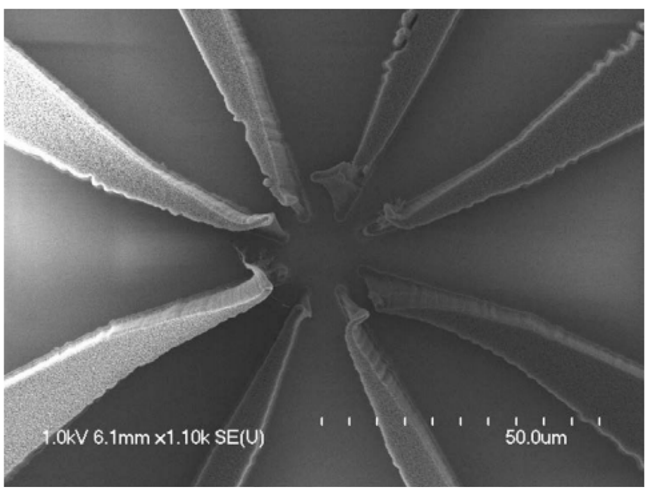
Bottom: Simulation result shows agreement with experiments.

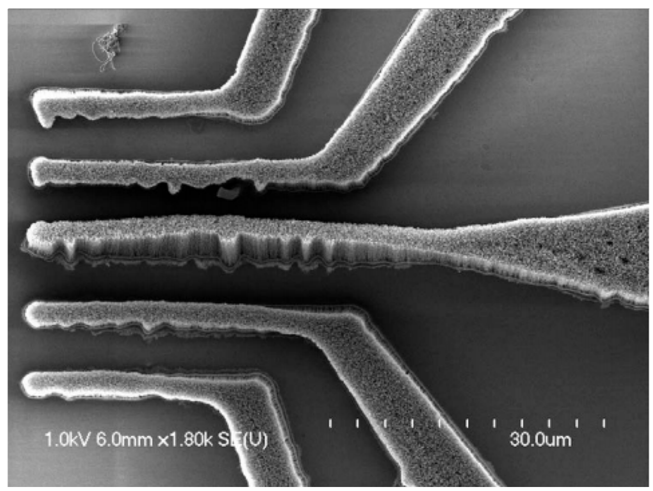
Vertically-Aligned Carbon-Nanotubes Embedded in Ceramic Matrices for Hot Electrode Applications

Performer	University of Nebraska
Award Number	FE0023061
Project Duration	10/01/2014 – 09/30/2018
Total Project Value	$ 400,000
Technology Area	University Training and Research

NETL is partnering with the University of Nebraska to develop carbon nanotube (CNT)-ceramic composite structures in which vertically aligned carbon nanotubes are embedded in ceramic matrices for hot electrode applications such as magnetohydrodynamic (MHD) power systems. Four objectives will be accomplished: (1) super growth of vertically aligned CNT carpets, (2) fabrication of CNT-boron nitride (BN) composite structures, (3) stability and resistance studies of the CNT-BN composite structures, and (4) thermionic emissions from the CNT-BN composite structures. The research team will grow vertically aligned (up to 1 cm thick) carbon nanotube carpets on copper.

Successful development of the CNT ceramic composite structures will reduce the capital costs of MHD power systems and establish a new family of vertically aligned CNT-based anisotropic composite structures.





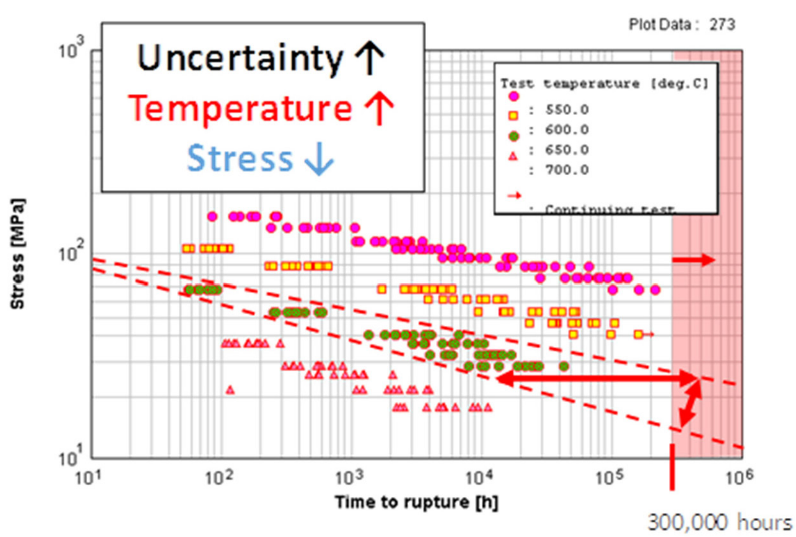
Vertically aligned CNT patterns: two potential models of the carbon dispersion within the SiC bulk.

An Accelerated Creep Testing Program for Advanced Creep Resistant Alloys for High Temperature Fossil Energy Applications

Performer	University of Texas at El Paso
Award Number	FE0030331
Project Duration	09/01/2017 – 08/31/2020
Total Project Value	$ 400,000
Technology Area	Plant Optimization Technologies

NETL is partnering with the University of Texas at El Paso to vet, improve, and test the feasibility of accelerated creep testing (ACT) for metallic materials. These overarching goals will be achieved by the following technical approach. A database of long-term creep data for surrogate materials P91 steel and IN718 nickel-based superalloy will be collected. Pre-ACT experiments will be performed to establish the baseline properties of the material, evaluate a reference-calibration approach for the ACTs, and develop creep deformation mechanisms map. The framework of the ACTs will be scrutinized and mathematical rules and constraints posed to establish the systematic repeatability of time acceleration. A targeted test matrix of ACTs will be executed to probe the limits of time acceleration. A post-audit validation where ACT tests are compared to the experimental database will be used to determine the extent that the ACTs are independent of systematic errors and calibration bias. Finally, a comprehensive American Society for Testing and Materials style “Test Standard - An Accelerated Creep Testing Program for New Material Qualification” will be written that includes geometry, test parameters, regression software, and recommendations for the retrofit of existing creep frames.

This project has the potential to reduce the time to implementation of new creep resistant alloys from decades to months. The ACTs could enable the collection of multistage creep deformation and rupture of extremely long-lived (106 hours) metallic materials in less than 24 hours. The outcome of this study will be an accelerated creep testing program for new material qualification. Original equipment manufacturers and plant owners can then use this knowledge to design and predict the remaining life of fossil energy components with more reliability.



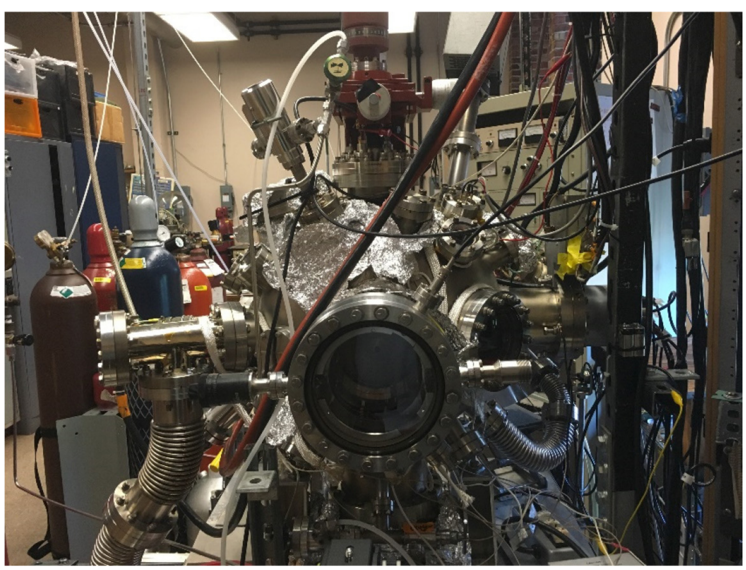
Creep-rupture of 9Cr-1Mo tube.

Precursor-Derived Nanostructured Silicon Carbide Based Materials for Magnetohydrodynamic Electrode Applications

Performer	University of Washington
Award Number	FE0023142
Project Duration	10/01/2014 – 09/30/2018
Total Project Value	$ 399,989
Collaborator	Clemson University
Technology Area	University Training and Research

NETL is partnering with the University of Washington (UW) to develop a novel class of SiC-based ceramic composite materials through a polymer-precursor-derived route with tailored compositions for channel applications in magnetohydrodynamic (MHD) generators. UW will investigate the effect of precursor chemistry (specifically C/Si) and processing conditions (e.g., temperature) on the nanodomain structure, resultant stoichiometry, nature of the carbon phase (e.g., graphene sheets, carbon nanoparticles), and the resulting thermo-mechanical properties at elevated temperatures. A minor constituent 'X' in Si-C-X is incorporated at the precursor stage during material synthesis, and its effect on the electrical properties, including electrical conductivity, thermionic emissions, and arcing properties for use in MHD generators will be investigated. Important parameters to be investigated are the domain size, the type and distribution of carbon, and the sizes and volume fractions of crystalline SiC and the constituent X. UW will also investigate the interaction of these materials with plasma as a first step toward understanding the plasma-induced degradation process using a newly developed High Density Plasma-Materials Testing Facility that was designed and built on the UW campus.

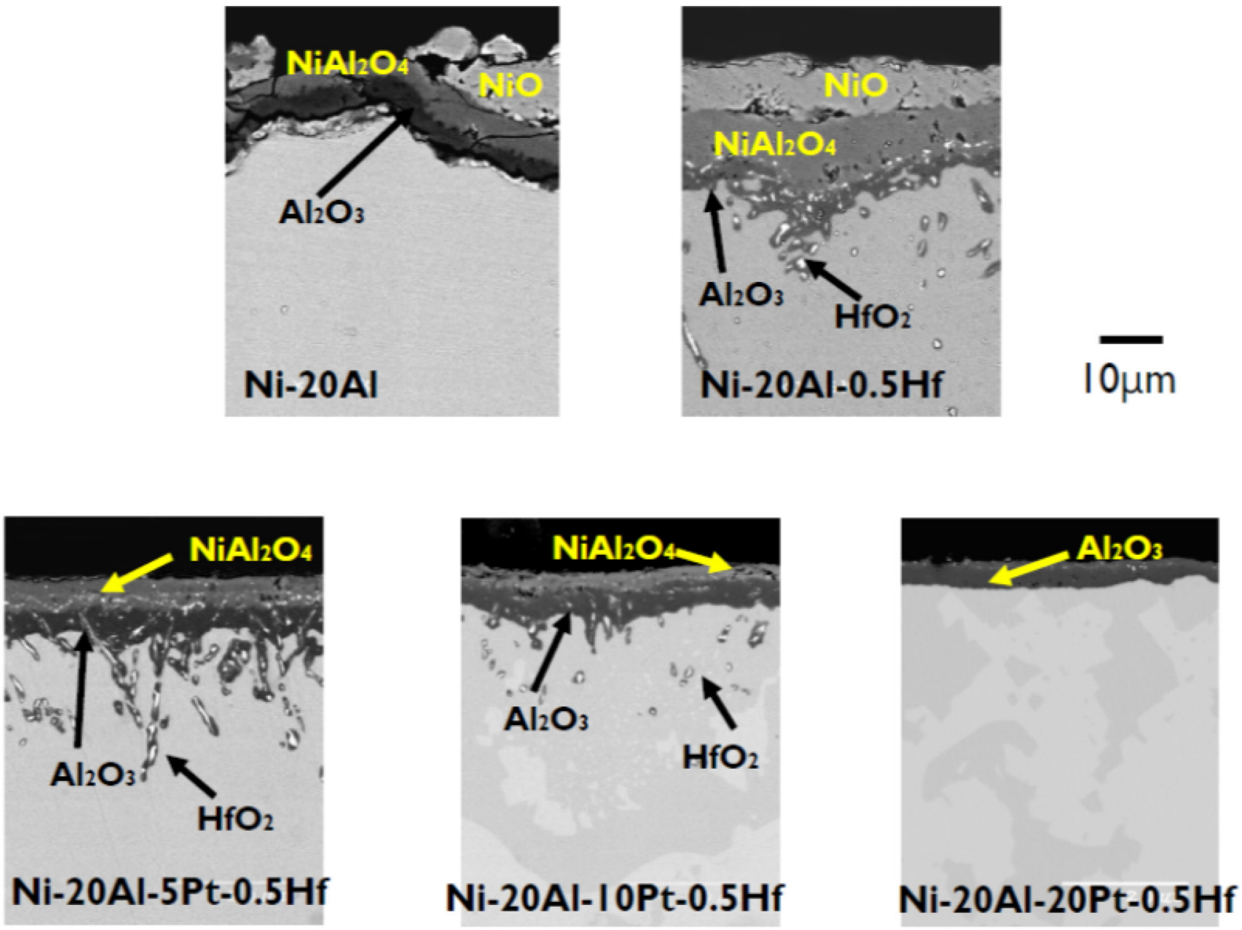
By developing SiC-based materials with nanostructured features and tailoring their compositions, the high-temperature resistance, electrical properties, and plasma resistance of SiC will improve relative to that of SiC produced by conventional powder processing approaches such as solid state sintering. A successful outcome of this research will result in the emergence of reliable and affordable designed materials for MHD applications.



Front view of electron grid.

COMPUTATIONAL MATERIALS MODELING

The objective of Computational Based Materials Design and Performance Prediction is to enable rapid design of new high performance materials, and provide validated models capable of simulating and predicting long-term performance of high performance materials.



Cross-sectional images of Ni-20at %Al-Pt-Hf γ/γ' alloys after 500 oxidation cycles at 1150 °C in air.

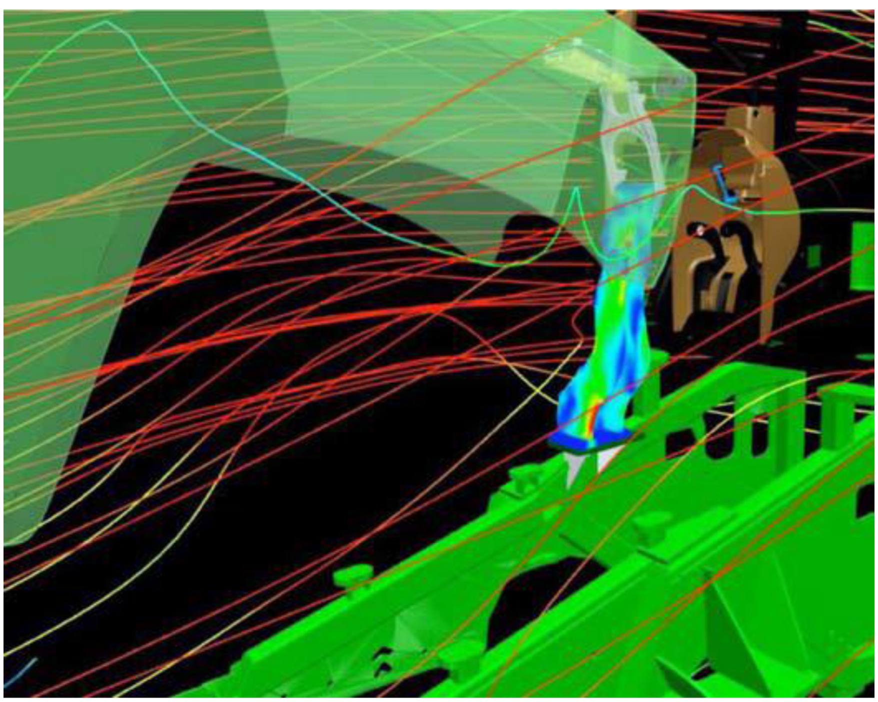
Computational System Dynamics (Computational Design of Multiscale Systems)

Performer	Ames National Laboratory
Award Number	FWP-AL-14-450-012
Project Duration	10/01/2014 – 09/30/2018
Total Project Value	$791,000
Technology Area	Coal Utilization Sciences

NETL is partnering with Ames National Laboratory to develop computational algorithms, strategies, and an informational framework needed to design materials in an integrated manner across length and time scales, creating the ability to design and tailor material properties for specific applications. The overall objective of the project is to provide a capability to assess degradation mechanisms and improve the reliability of refractory alloys for coal gasification and related processes.

The project will investigate potential alloy formulations using progressively more accurate thermodynamic methods; conduct critical experiments to test the accuracy of the calculations; evaluate each alloy's key mechanical, thermal, and oxidation properties; and screen alloys showing the greatest potential for high performance thermochemical stability using state-of-the-art thermal analysis, high-temperature X-ray diffraction analysis, and microstructural evaluation with electron microscopy.

The resulting tool will allow researchers to reduce possible alloy formulations from tens of thousands to a manageable number of combinations that are most likely to succeed.



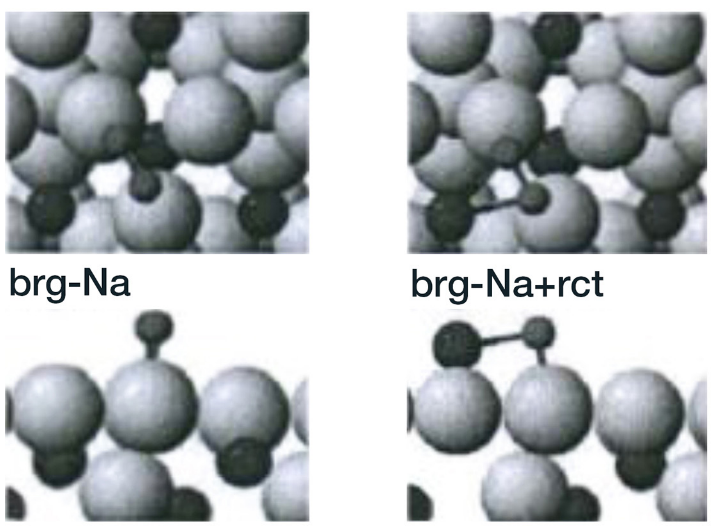
Graphic output from Virtual Engineering (VE) -suite of a simulation of the response of part of a component to an external load.

The SMARTER Project (Science of Multicomponent Alloys: Roadmap for Theoretical and Experimental Research)

Performer	Ames National Laboratory
Award Number	FWP-AL-14-510-075
Project Duration	04/01/2015 – 09/30/2018
Total Project Value	$ 510,000
Technology Area	Coal Utilization Sciences

NETL is partnering with Ames National Laboratory to propose a new methodology to speed the discovery and optimization of chemically complex alloys and to leverage theoretical and experimental capabilities for assessing their long-term stability. Near equiatomic alloys have a high degree of chemical disorder in a single high-temperature (T) phase leading to high mechanical strength. These disordered alloys have potential for fossil energy use in high-T applications; however, their long-term stability in harsh combustion environments has not yet been explored.

Near equiatomic alloys offer excellent promise as structural materials for use in several commercial applications, including gas turbines for power generation, advanced ultrasupercritical boiler walls, aerospace engines, and nuclear reactor walls.



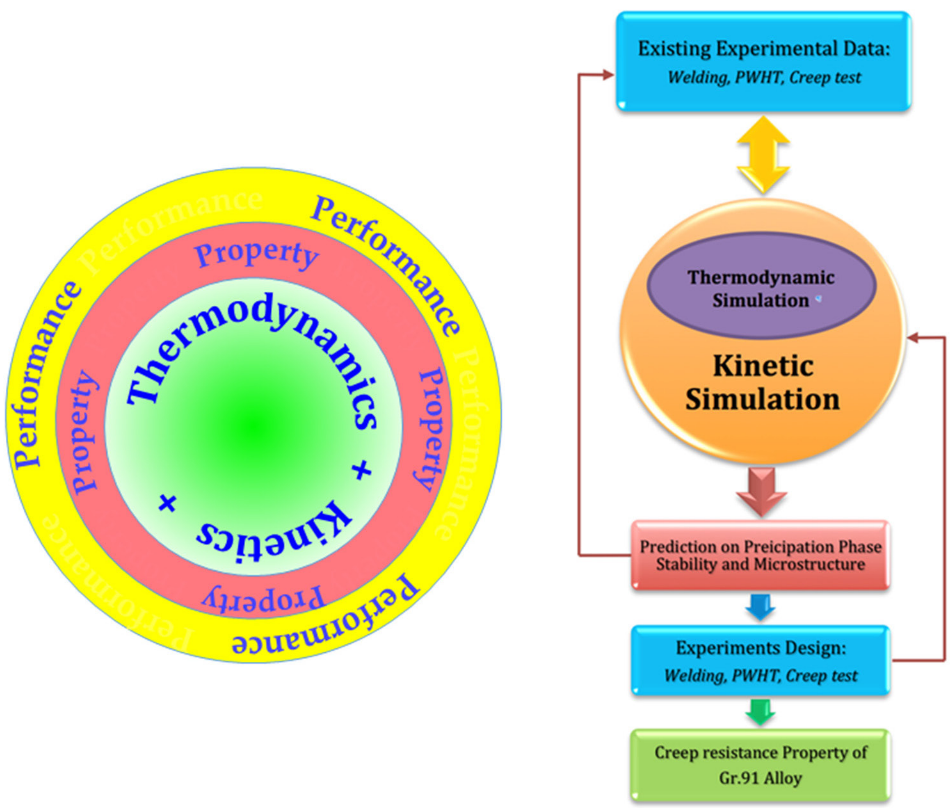
O_2 adsorption on $NaAu_2$ (111) surface at the brg-Na site (left) and the same site with reconstruction of surface Na pop-up (right).

The Fundamental Creep Behavior Model of GR.91 Alloy by Integrated Computational Materials Engineering (ICME) Approach

Performer	Florida International University
Award Number	FE0027800
Project Duration	08/01/2016 – 07/31/2019
Total Project Value	$ 250,000
Collaborator	Ohio State University
Technology Area	University Training and Research

NETL is partnering with the Florida International University to investigate the fundamental creep cracking mechanism of the Gr.91 alloy under advanced power generation operating conditions to establish links among composition, processing parameters, phase stability, microstructure, and creep resistance using the ICME approach. Specifically, the project team will predict the phase stability and microstructure of Gr.91 base alloy and weldment with the computational thermodynamics and kinetics–calculation of phase diagrams (CALPHAD) approach; perform welding, heat treatment, and creep testing of the Gr.91 alloy; develop a model that will provide an excellent match with experimental data from current and previous work on Gr.91. alloy; and predict how to improve the long-term creep resistance for the Gr.91 family of alloys.

The model will improve the creep resistance of Gr.91 alloys for use in advanced fossil-fueled power generation systems and other applications, thus increasing fossil-fueled power generation efficiency and reducing emissions.



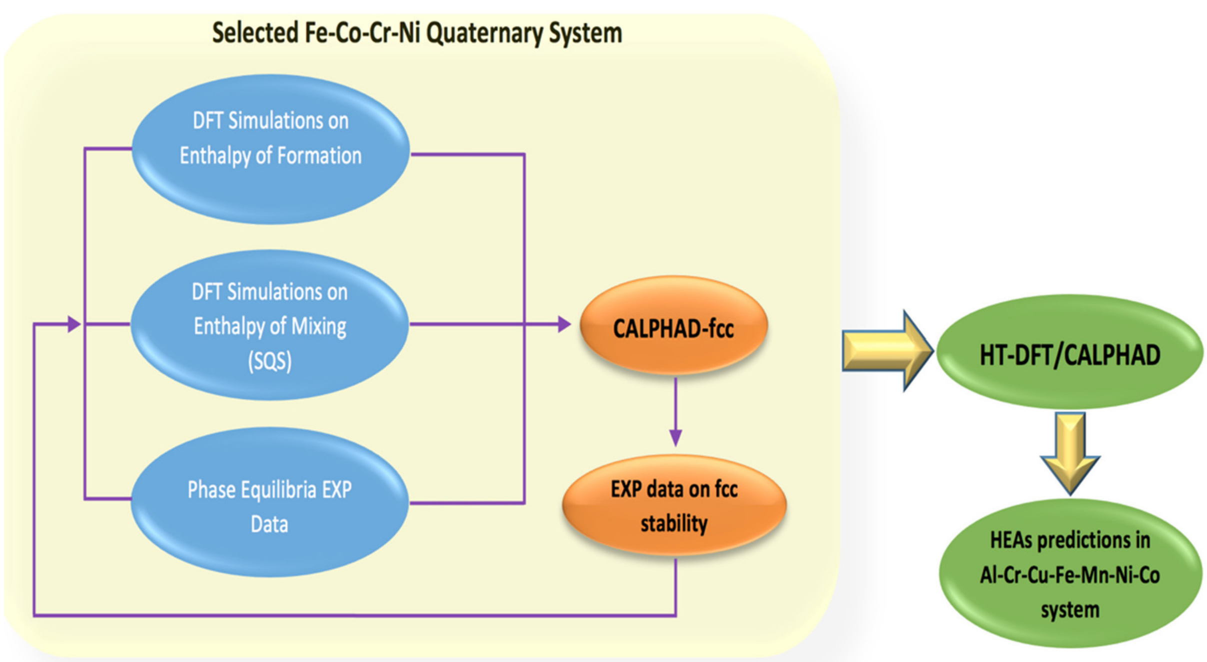
Materials design using ICME approach.

The Novel Hybrid Ab Initio Model of High Performance Structural Alloys Design for Fossil Energy Power Plants

Performer	Florida International University
Award Number	FE0030585
Project Duration	08/01/2017 – 07/31/2020
Total Project Value	$ 250,000
Technology Area	University Training and Research

The project team will develop an ab initio approach to quickly design new high-performance structural alloys for use in fossil energy power plants. The specific project objectives are to (1) conduct density functional theory (DFT) simulations for the selected Fe-Co-Cr-Ni quaternary system; (2) develop a thermodynamic database specifically for the face-centered cubic (FCC) phase of the selected system; (3) predict the compositions of new alloys in the selected system and compare them to experimental observations; (4) develop a hybrid high-throughput-DFT/CALPHAD model, which is capable of efficiently predicting the compositions of new alloys for multicomponent systems; and (5) apply the approach to make predictions on high-entropy alloys in an Al-Cr-Cu-Fe-Mn-Ni-Co multicomponent system.

The project will culminate in the development of a hybrid model based on high-throughput DFT simulations and computational thermodynamics to provide guidance on how to identify new multicomponent, high-performance structural alloys with much less computational effort. The model will address the extensive computational time needed for DFT when designing new alloys.



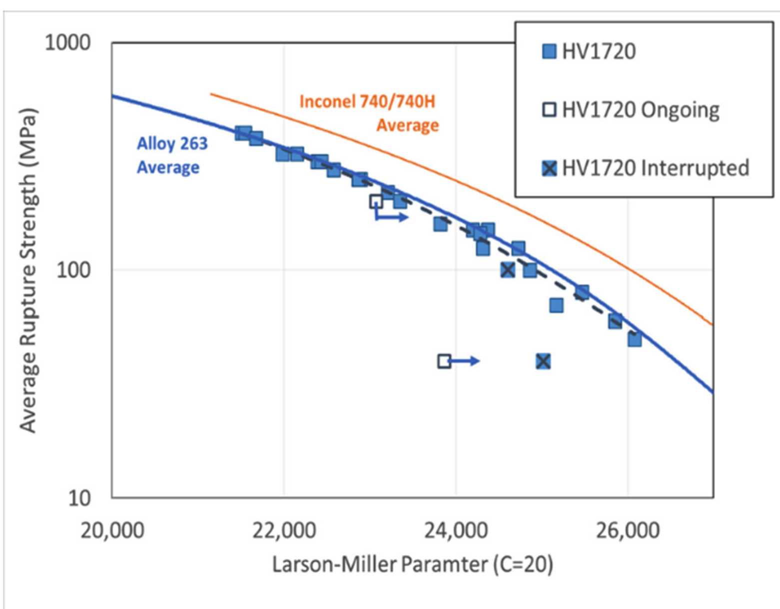
Development of the hybrid ab initio/CALPHAD approach.

Development of a Physically-Based Creep Model Incorporating Eta Phase Evolution for Nickel-Base Superalloys

Performer	Michigan Technological University
Award Number	FE0027822
Project Duration	08/15/2016 – 08/14/2019
Total Project Value	$ 399,996
Technology Area	University Training and Research

NETL is partnering with the Michigan Technological University to develop a physically based creep model for Nimonic 263 that synthesizes known creep behavior based on gamma prime strengthening to gain a new understanding of the effects of eta phase on creep performance at long service times in fossil energy power plants. This project team will develop heat treatments for commercial Nimonic 263 to obtain a mixture of both eta (η) and gamma prime (γ') phases prior to creep testing, with the γ' distribution being as close to commercial Nimonic 263 as possible; conduct creep tests on these materials at the Electric Power Research Institute; fully characterize microstructures and deformation mechanisms during creep for all three alloys (standard Nimonic 263, Nimonic 263 heat-treated to contain $\eta + \gamma'$, and the Michigan Tech modified Nimonic 263 alloy that contains only eta); and use the knowledge gained to develop and validate a physically-based creep model that synthesizes known gamma prime creep behavior to gain a new understanding of the effects of eta phase on creep performance.

The results will enhance life prediction, component design, and alloy selection for advanced fossil energy power plant systems.



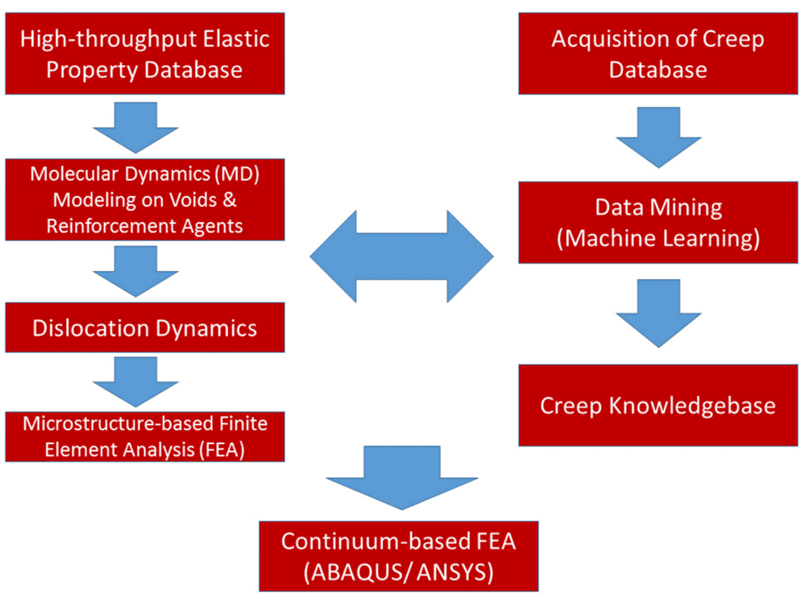
Alloy 20, Widmanstätten microstructure, creep.

Multimodal Approach to Modeling Creep Deformation in Nickel-base Superalloys

Performer	Missouri State University
Award Number	FE0031554
Project Duration	12/15/2017 – 12/14/2020
Total Project Value	$ 918,370
Collaborators	Missouri University of Science and Technology and University of Missouri - KC
Technology Area	Plant Optimization Technologies

NETL is partnering with Missouri State University to develop a new multi-modal approach to modeling of creep deformation in nickel-base superalloys. The approach is based on a two-pronged strategy combining a bottom-up, multi-scale, physically-based modeling approach and a data-mining-driven top-down approach, backed by experimental database and correlation connectivity with strength augmented by data mining/machine learning protocols. The overarching goal is to integrate these two strategies to create quantitatively better predictive creep models that are not only sensitive to the microstructural evolution during various stages of creep, but also based on physically sound creep modeling that judiciously encompasses the strength of each modeling scale and provides a more comprehensive creep deformation analysis via finite element analysis.

The main advantage of the project's approach is to establish a new framework within which the adaptation of data mining tools for predicting the creep property of nickel-base alloys can be accelerated using a rigorous step-by-step atomistic-mesoscale-continuum based simulation. This approach will reduce the level of uncertainty of experimental creep data and facilitate a better linkage between the experimentally-acquired creep data and the creep models that are established through the hierarchical multi-scale modeling. Ultimately, it will provide better diagnostics on the slow progression of creep deformation and will help to improve the quantitative predictive capability for the onset of creep failure during the tertiary creep stage. The approach can also be applied to a wider range of material candidates for fossil energy power plants.



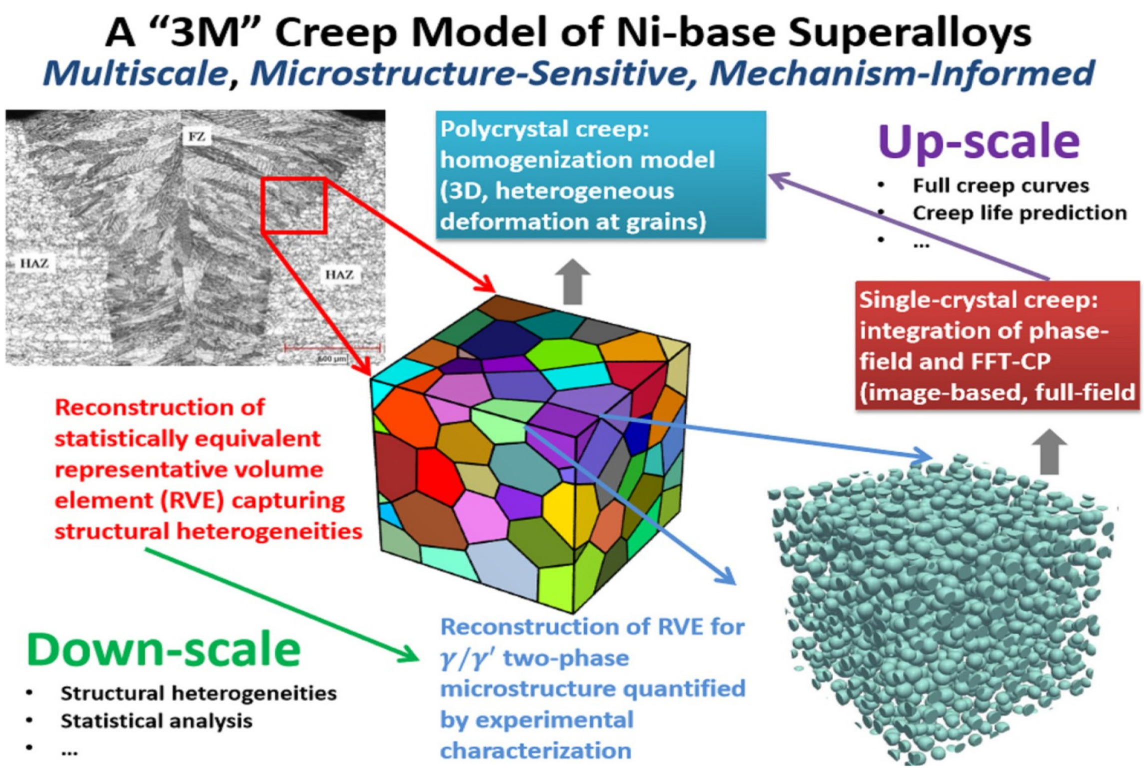
Schematics of overall multi-modal workflow of proposed new roadmap to integrate the use of experimental creep database ("top-down" approach) with multi-scale modeling ("bottom-up" approach).

ICME for Creep of Ni-base Superalloys in Advanced Ultra-Supercritical Steam Turbines

Performer	Ohio State University
Award Number	FE0027776
Project Duration	09/01/2016 – 07/31/2019
Total Project Value	$ 400,000
Technology Area	University Training and Research

NETL is partnering with Ohio State University to combine materials informatics and physics based modeling for an integrated computational materials engineering (ICME) approach to predict long-term creep behavior of nickel (Ni)-based superalloys for advanced ultrasupercritical (AUSC) steam turbine applications. This project will apply advanced materials informatics for critical assessment of existing experimental data from creep tests on selected alloys; evaluate existing models to ascertain confidence in creep-life predictions and determine which, if any, provide a statistically adequate fit to and safe extrapolation of the data; and develop new modeling capabilities needed to predict long-term creep behavior of Ni-based superalloys for use in AUSC coal-fired power plant steam turbines.

This project will assess the long-term creep performance of Ni-based superalloys more accurately and efficiently, accelerate development and qualification of new materials for next generation AUSC steam turbine systems, and increase the efficiency and reduce the emissions of coal-fired power plants.



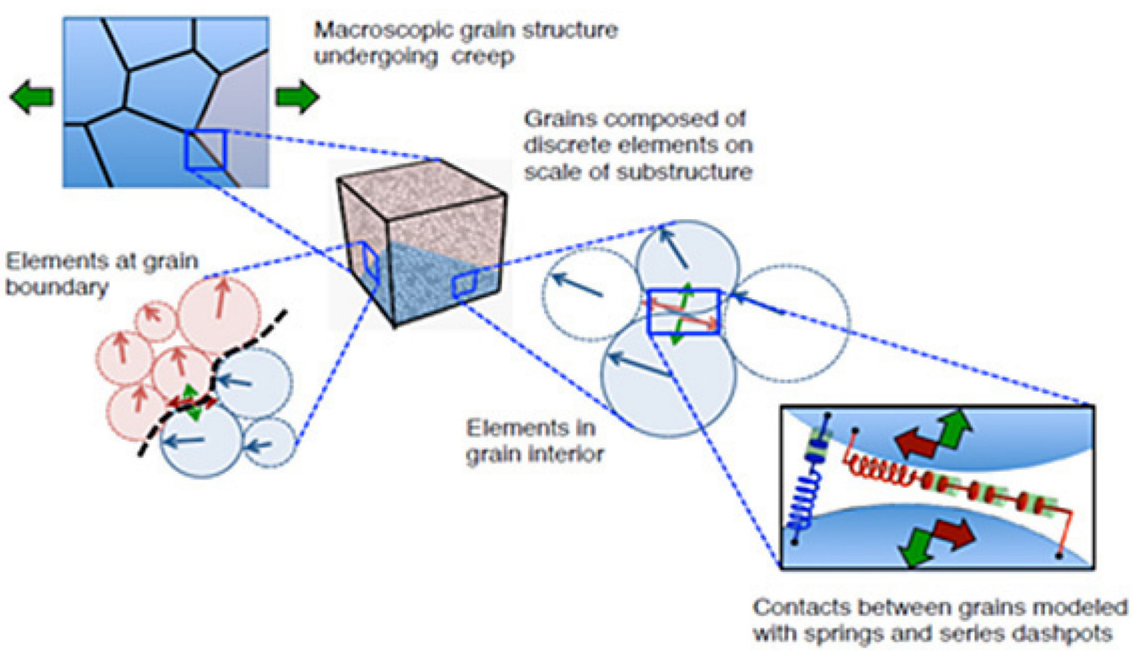
ICME approach.

New Mechanistic Models of Long Term Evolution of Microstructure and Mechanical Properties of Nickel Based Alloys

Performer	Oregon State University
Award Number	FE0024065
Project Duration	01/01/2015 – 12/31/2017
Total Project Value	$ 624,999
Technology Area	Coal Utilization Sciences

NETL is partnering with Oregon State University to create and validate a robust multiscale, mechanism-based model that quantitatively predicts long-term evolution of microstructure for nickel-based alloys as well as the effect on mechanical properties such as creep and rupture strength, including variable cyclic operating conditions.

Mechanism-based modeling has the potential to simulate long-term behavior (10–30 years) based on shorter time data (diffusion constants, activation energies, etc.) to achieve greater confidence in long-term life, safer and more cost-efficient designs, ability to better predict variable operating conditions, and extended service life beyond initial assumptions.



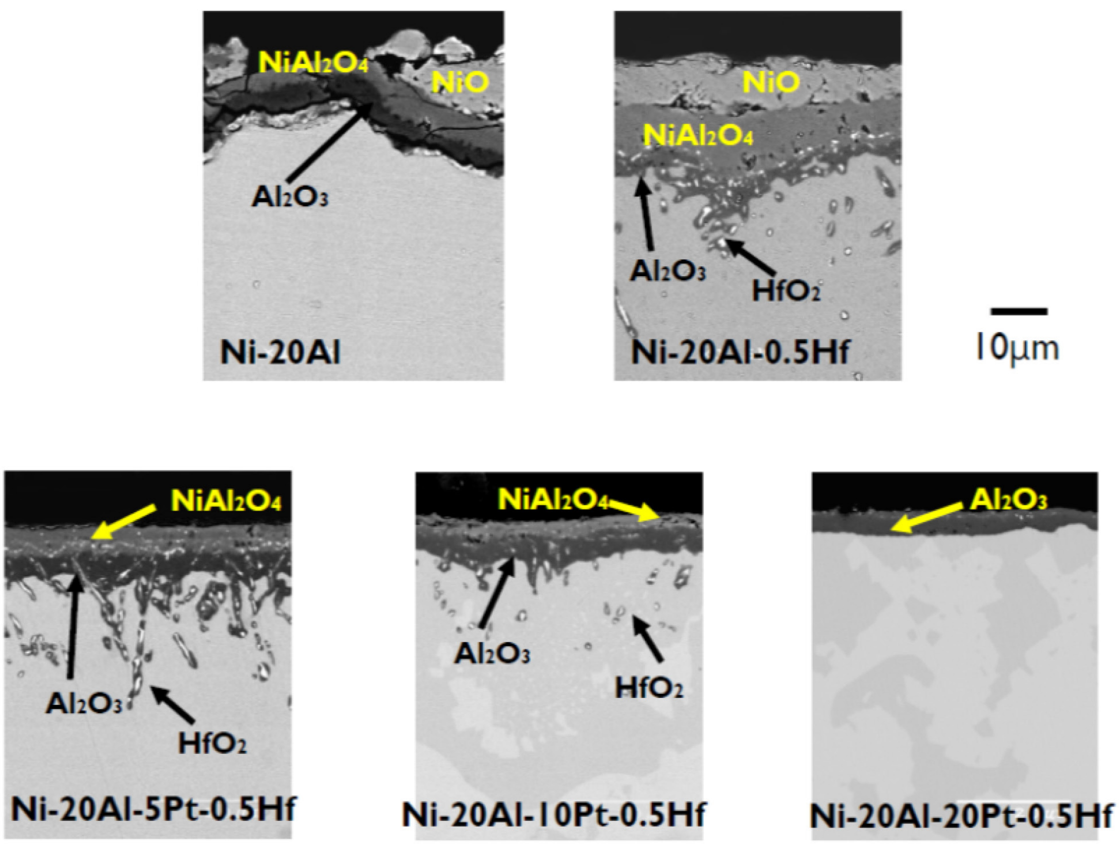
Schematic representation of the proposed DEM model. Crystal grains will be represented using discrete elements that interact and move to allow deformation and microstructure evolution. The element interaction laws will be defined to represent the physical mechanisms involved for nickel based alloys

Computational Design and Discovery of Ni-based Alloys and Coatings: Thermodynamic Approaches Validated by Experiments

Performer	Pennsylvania State University
Award Number	FE0024056
Project Duration	01/01/2015 – 10/31/2017
Total Project Value	$ 632,176
Collaborator	University of Pittsburgh
Technology Area	Coal Utilization Sciences

NETL is partnering with Pennsylvania State University to develop a thermodynamic foundation for the accelerated design of nickel-based alloys and coatings. The information derived will be essential for efficiently designing and predicting the performance of alloys, coatings, and coating/alloy combinations. The project will also develop an automated thermodynamic modeling tool that will more efficiently arrive at accurate thermodynamic descriptions and enhance computational alloy and coating design.

The project's resulting database will enable prediction of tunable properties (including phase compositions and fractions), solubility limits, and driving forces—all of which are important in designing high-temperature alloys and coatings that have long-term resistance to harsh service environments.



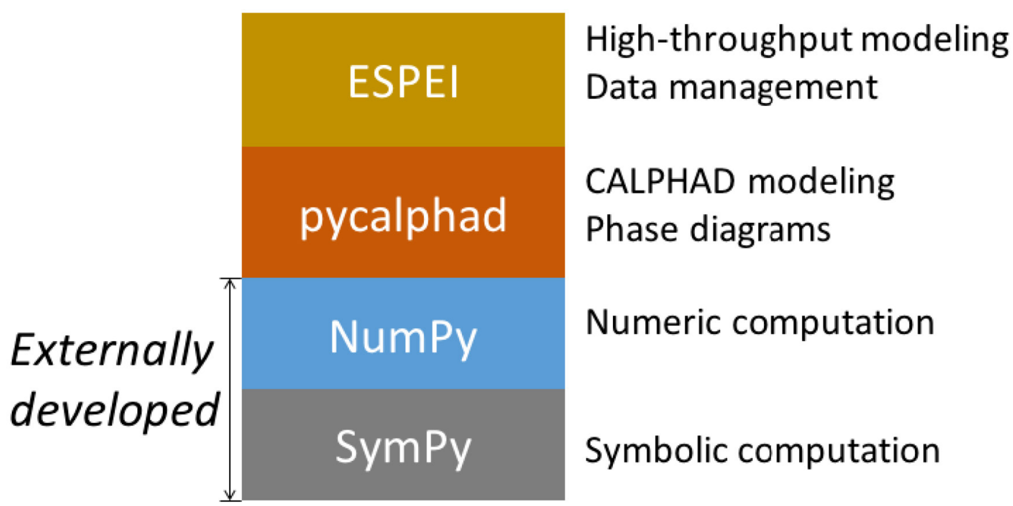
Cross-sectional images of Ni-20at %Al-Pt-Hf γ/γ' alloys after 500 oxidation cycles at 1150 °C in air.

High Throughput Computational Framework of Materials Properties for Extreme Environments

Performer	Pennsylvania State University
Award Number	FE0031553
Project Duration	12/15/2017 – 12/14/2020
Total Project Value	$ 937,836
Technology Area	Plant Optimization Technologies

NETL is partnering with Pennsylvania State University to establish a framework capable of efficiently predicting the properties of structural materials for service in harsh environments over a wide range of temperatures and over long periods of time. The approach will be to develop and integrate high-throughput first-principles calculations based on density functional theory in combination with machine learning methods, perform high throughput calculation of phase diagrams (CALPHAD) modeling, and carry out finite-element-method simulations. In regard to high-temperature service in fossil power systems, nickel-based superalloys Inconel 740 and Haynes 282 will be investigated.

The framework has the potential to enable high-throughput computation of tensile properties of multi-component alloys at elevated temperatures, resulting in significant reduction in computational time needed by the state-of-the-art methods. Once successfully completed, the project will deliver an open-source framework for high-throughput computational design of multi-component materials under extreme environments. This framework will enable more rapid design of materials and offer the capability for further development of additional tools due to its open-source nature.



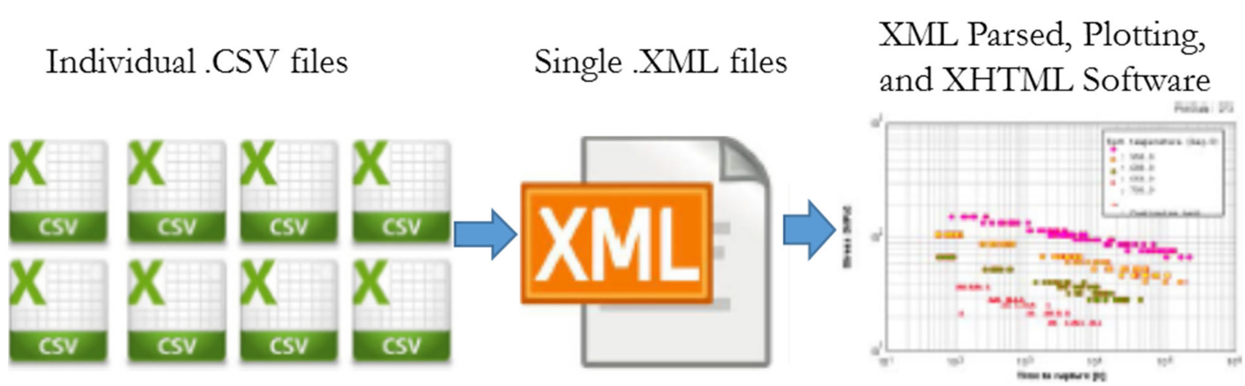
ESPEI-2.0 software stack.

A Guideline for the Assessment of Uniaxial Creep and Creep-Fatigue Data and Models

Performer	University of Texas at El Paso
Award Number	FE0027581
Project Duration	09/01/2016 – 08/31/2019
Total Project Value	$ 250,000
Technology Area	University Training and Research

NETL is partnering with the University of Texas at El Paso to develop an aggregated database of creep and creep-fatigue validation data from existing datasets for P91 steel and 316 stainless steel. Specifically, the project will benchmark the creep and creep-fatigue modeling results obtained into a variety of finite element models; evaluate and test the performance of the models with respect to experimental uncertainty and the repeatability and stability of extrapolations across boundary conditions and regimes; computationally validate and assess creep and creep-fatigue constitutive models for standard and non-standard loading conditions; and expand the University of Texas at El Paso's capability to conduct experimental research that replicates the extreme boundary conditions experienced by modern and advanced materials.

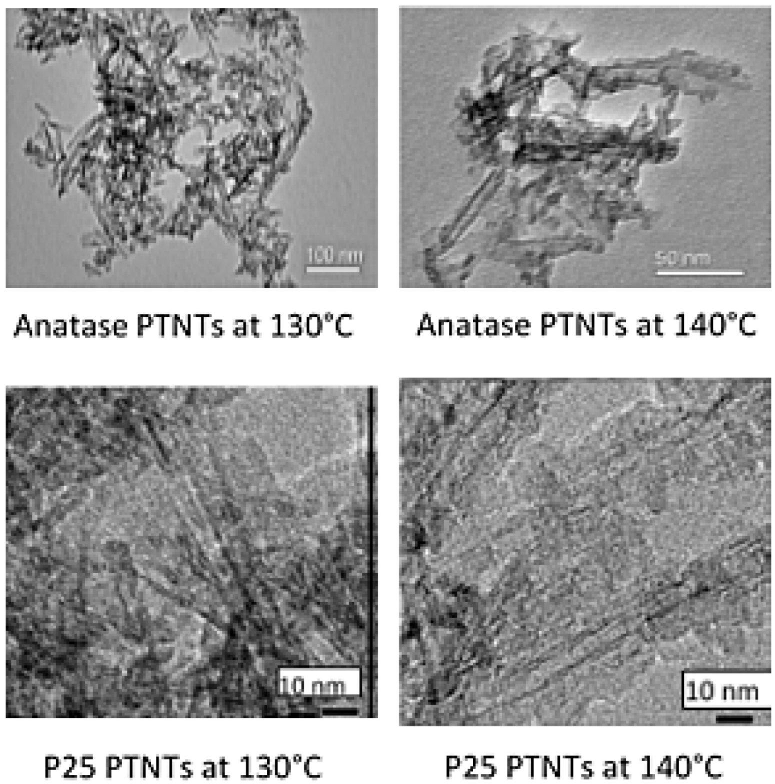
A component designer will be able to use the resulting guidelines to easily select the best constitutive model(s) and experimental datasets for intended designs.



Extensible markup language (XML) database structure.

FUNCTIONAL MATERIALS

The objective of Functional Materials for Process Performance Improvements is to develop functional materials such as sorbents, coatings, catalysts, chemical-looping oxygen carriers, and high-temperature thermo-electrics needed for advanced FE power generation technologies.



Transmission electron microscopy results.

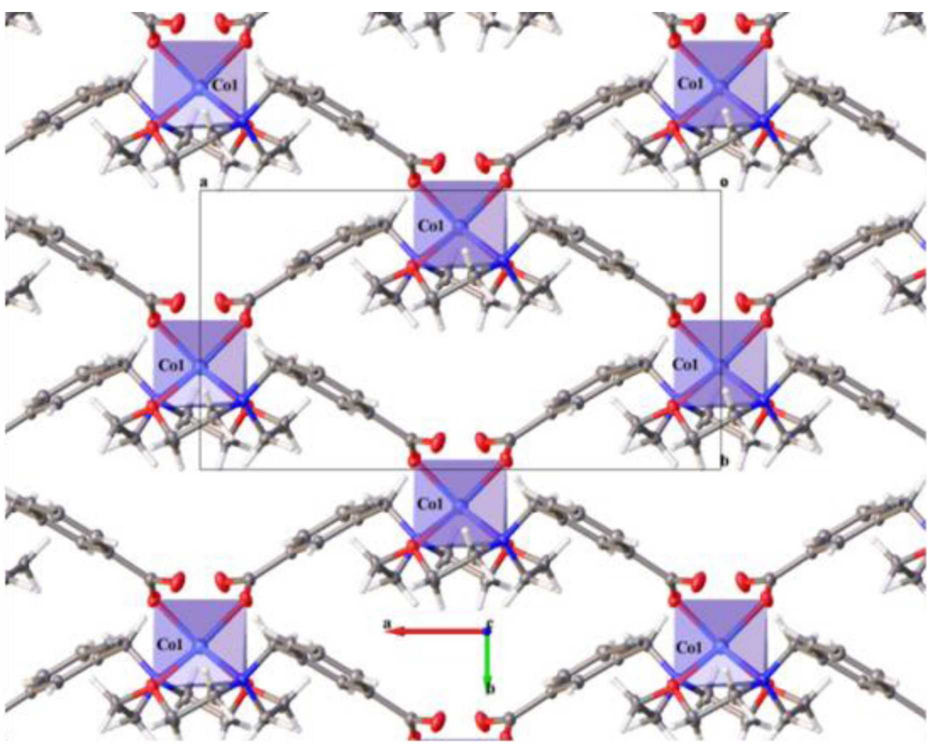
PERFORMER	PROJECT TITLE	PAGE
Clark Atlanta University	Engineering Accessible Adsorption Sites in Metal Organic Frameworks for CO_2 Capture	52
Pennsylvania State University	University Coalition for Fossil Energy Research	53
Prairie View A&M University	Post Combustion Carbon Capture Using Polyethylenimine (PEI) Functionalized Titanate Nanotubes	54
University of Tennessee Space Institute	Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage	55
West Virginia University Research Corporation	Ceramic High Temperature Thermoelectric Heat Exchanger and Heat Recuperators in the Power Generation Systems	56

Engineering Accessible Adsorption Sites in Metal Organic Frameworks for CO_2 Capture

Performer	Clark Atlanta University
Award Number	FE0022952
Project Duration	10/01/2014 – 09/30/2018
Total Project Value	$ 249,998
Technology Area	University Training and Research

NETL is partnering with Clark Atlanta University (CAU) to synthesize metal organic frameworks (MOFs) with improved site accessibility and thus enhanced carbon dioxide (CO_2) adsorption and selectivity properties. CAU will synthesize and characterize ultra-high-surface-area MOF materials for CO_2 adsorption. This three-year research effort will consist of synthesizing MOFs with organic linkers as well as nitrogen-containing pyrazine linkers and evaluate them based on their CO_2 adsorption properties, framework structure and composition (such as metal content and elemental analysis), surface area, pore size, and thermal stability. The evaluation methods will include X-ray crystallography, powder X-ray diffraction, thermogravimetric analysis, infrared spectroscopy, and other advanced techniques. The downselected CO_2 adsorption material from this research will be used for CO_2 capture and sequestration applications.

The proposed research supports the Department of Energy Office of Fossil Energy and the National Energy Technology Laboratory mission by advancing the science of coal/fossil fuel technologies, specifically carbon capture. The research will guide rational design and synthesis strategies toward producing advanced sorbents for CO_2 capture. Successful CO_2 adsorbent materials can potentially have an industrial and environmental impact. This project will also provide research opportunities for students in the fields of chemistry and materials science related to the use of fossil energy resources.



2D cobalt- diazo crown ether carboxylate metal oxide framework. Ingram et al. 2013, Crystal Growth and Design.

University Coalition for Fossil Energy Research

Performer	Pennsylvania State University
Award Number	FE0026825
Project Duration	10/01/2015 – 09/30/2021
Total Project Value	$ 20,000,000
Technology Area	Post-Combustion Capture

The University Coalition will bring together a multi-disciplinary team of researchers from numerous universities to address fundamental research challenges to the advancement of fossil energy-based technologies. Work conducted through the Coalition will be technically aligned and complementary to the Office of Fossil Energy's (FE) goals and objectives. Research efforts will directly support FE's Strategic Center for Coal and the Strategic Center for Natural Gas and Oil in a variety of program areas including advanced energy systems, CO2 capture and storage, natural gas resources and infrastructure, and onshore and offshore oil and gas technology. The research completed under the initiative is expected to accelerate the development and deployment of fossil-fuel-based technologies to enable continued use of our nation's abundant natural resources in a cost effective and environmentally responsible manner.

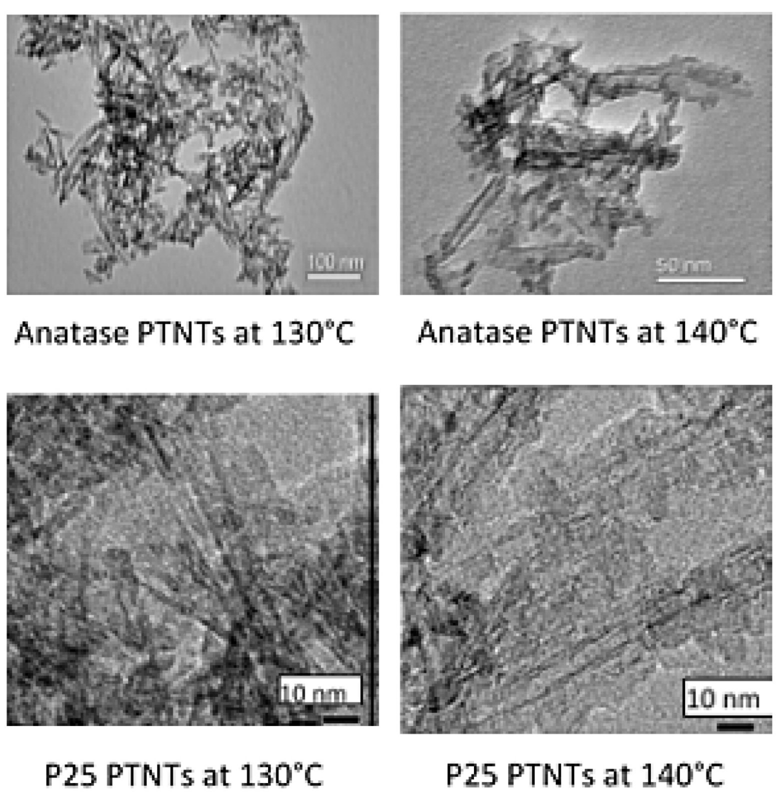
Project focuses on advancing basic and applied energy research.

Post Combustion Carbon Capture Using Polyethylenimine (PEI) Functionalized Titanate Nanotubes

Performer	Prairie View A&M University
Award Number	FE0023040
Project Duration	10/01/2014 – 09/30/2018
Total Project Value	$ 249,996
Technology Area	University Training and Research

NETL is partnering with Prairie View A&M University to develop a novel nanomaterial to efficiently capture CO_2 from the flue gas of fossil energy power generation systems by (1) establishing a knowledge base for the synthesis of titanium dioxide (TiO_2) nanotubes and adsorption characteristics of polyethylenimine (PEI) as well as the various protocols available for the impregnation of PEI; (2) characterizing the impregnated nanotubes and using them for refining synthesis parameters such as temperature, concentration, and time; (3) developing computational fluid dynamic (CFD) simulations in order to optimize the reactor conditions for high carbon capture efficiency; (4) demonstrating the carbon capture efficiency of impregnated TiO_2 tubes under various environmental conditions such as temperature and concentration; and (5) establishing a validated CFD model and a standard operating procedure for carbon capture using PEI impregnated TiO_2 nanotubes. Research will optimize the procedures for synthesizing the nanotubes and the impregnation protocols and develop standard operating procedures for carbon capture at different temperatures and concentrations.

A successful outcome from the study could be development of a high-efficiency, low-cost method to capture CO_2 from effluents of advanced fossil energy systems.



Transmission electron microscopy results.

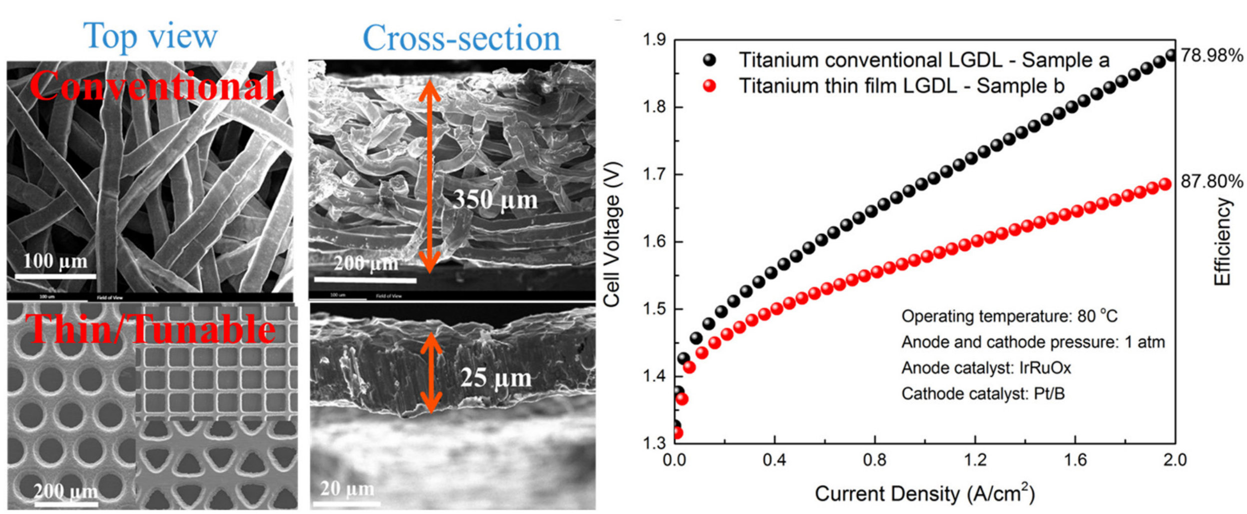
Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage

Performer	University of Tennessee
Award Number	FE0011585
Project Duration	09/01/2013– 08/31/2018
Total Project Value	$ 470,084
Technology Area	University Training and Research

NETL is partnering with the University of Tennessee to develop a thin and well-tunable multifunctional component via micro/nano fabrication for high-efficiency electrical energy storage, which is critical for the long-term utilization of coal in energy applications to provide reliable, affordable electricity and modernize the electrical grid.

Novel titanium liquid/gas diffusion layers (LGDLs) with well-tunable pore morphologies were developed by employing micro/nano-manufacturing and showed significant performance improvements in proton exchange membrane electrolyzer cells (PEMECs). As shown in the figure below, the operating voltages required at a current density of 2.0 amps per centimeter squared for the LGDLs were as low as 1.69 volts, and efficiency reached a reported high of nearly 88 percent. In addition, the reduction in LGDL thickness from the 350 micrometers (μm) of conventional LGDLs to 25 μm will substantially reduce the weight and volume of PEMEC stacks, which can lead to new avenues for future development of low-cost and higher-performance PEMECs. The well-tunable features of LGDL including pore size, pore shape, pore distribution, and thus porosity and permeability, will be valuable in developing PEMEC models and validating simulations of PEMECs with optimal and repeatable performance.

This project will further optimize novel multifunctional materials to promote the efficiency of energy storage technologies. Improvements to energy storage technologies will promote improved utilization of power plant assets that can provide operational flexibility and result in lower capital and operating costs.



Left: Scanning electron microscopy images of conventional and thin/ well-tunable titanium multifunctional liquid/gas diffusion layers.

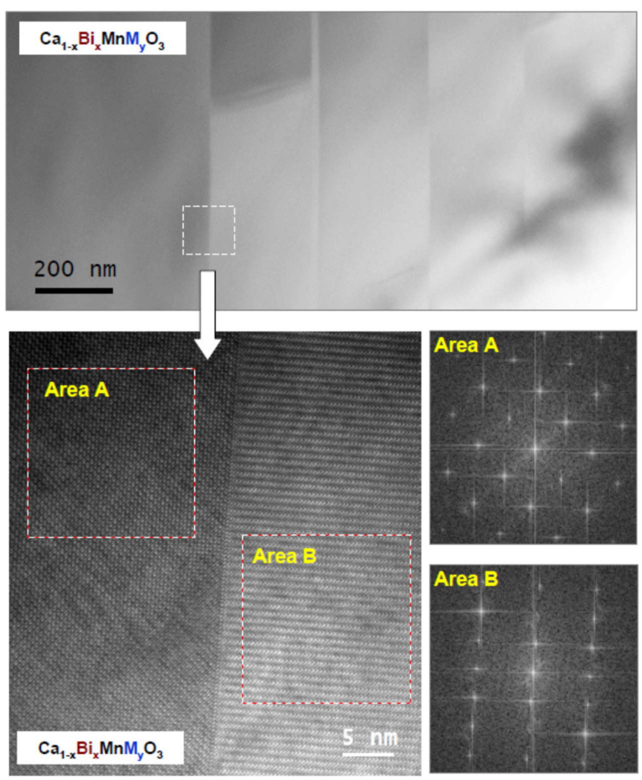
Right: Performance enhancement with the developed material.

Ceramic High Temperature Thermoelectric Heat Exchanger and Heat Recuperators in the Power Generation Systems

Performer	West Virginia University Research Corporation
Award Number	FE0024009
Project Duration	10/01/2014 – 03/31/2018
Total Project Value	$ 627,160
Technology Area	Plant Optimization Technologies

NETL is partnering with West Virginia University Research Corporation to develop compact and highly efficient all-oxide ceramic thermoelectric (TE) generators to work as compact heat exchangers and simultaneously recover the high-temperature waste heat from high-temperature power systems such as solid oxide fuel cells (SOFCs).

Combining the enhanced performance of oxide materials and the innovative designs of TE generators, the proposed all-oxide TE device will potentially over-perform state-of-the-art TE materials that are made of conventional metallic or semiconductor materials for high-temperature applications. The TE devices proposed in this project will be highly efficient, lightweight, reduced in size, highly stable in air at high temperatures, and non-toxic for powering sensors at temperatures in the 600 to 980 degrees Celsius range. In addition, the new devices will be easy to fabricate and thus will facilitate mass production with a high potential for use in large-scale operations. The incorporation of TE devices into SOFC systems is expected to increase electricity production by more than 15 percent, corresponding to system electrical efficiency increases of five percentage points.



No further crystal defects in calcium bismuth manganese oxide.

ABBREVIATIONS

°C . . . . . degrees Celsius
°F . . . . . degrees Fahrenheit
µm . . . . . micrometer
2D . . . . . two-dimensional
ACT . . . . . accelerated creep testing
AM . . . . . additive manufacturing
ASME . . . . . American Society of Mechanical Engineers
AUSC . . . . . advanced ultrasupercritical
CALPHAD . . . . . calculation of phase diagrams
CAU . . . . . Clark Atlanta University
CFD . . . . . computational fluid dynamics
cm . . . . . centimeter
CNT . . . . . carbon nanotubes
CO_2 . . . . . carbon dioxide
CSEF . . . . . creep strength enhanced ferritic
DEM . . . . . discrete element method
DFT . . . . . density functional theory
DOE . . . . . [U.S.] Department of Energy
EEM . . . . . extreme environment materials
FCC . . . . . face centered cubic
FE . . . . . [DOE Office of] Fossil Energy
FWP . . . . . Field Work Proposal
GB . . . . . grain boundary
GE . . . . . General Electric Company
H282 . . . . . Haynes 282
HBCU . . . . . Historically Black Colleges and Universities
HPM . . . . . high performance materials
hr . . . . . hour
HX . . . . . Hastelloy X
ICME . . . . . integrated computational materials engineering
ICWE . . . . . integrated computational weld engineering

ABBREVIATIONS

lb . . . . pound

LGDL . . . . liquid/gas diffusion layer

MHD . . . . magneto-hydrodynamic

MOFs . . . . metal organic framework

MW . . . . megawatt

NETL . . . . National Energy Technology Laboratory

NGO . . . . non-governmental organizations

NL . . . . national laboratory

ODS . . . . oxide dispersion strengthened

OMI . . . . Other Minority Institutions

ORNL . . . . Oak Ridge National Laboratory

PEI . . . . polyethylenimine

PEMEC . . . . proton exchange membrane electrolyzer cell

PNNL . . . . Pacific Northwest National Laboratory

psi . . . . pounds per square inch

psig . . . . pounds per square inch gauge (referenced to ambient)

R&D . . . . research and development

SBIR . . . . Small Business Innovation Research

sCO_2 . . . . supercritical carbon dioxide

SE&A . . . . systems engineering and analysis

SHS . . . . self-propagating high-temperature synthesis

SOFC . . . . solid oxide fuel cell

T . . . . temperature

TE . . . . thermoelectric

TMF . . . . thermomechanical fatigue

U.S. . . . . United States

UCR . . . . University Coal Research

UTR . . . . University Training and Research

UW . . . . University of Washington

VE . . . . virtual engineering

XML . . . . extensible markup language

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WEBSITES:

https://energy.gov/fe/plant-optimization-technologies#materials

http://www.netl.doe.gov/research/coal/crosscutting/high-performance-materials

ACKNOWLEDGEMENTS

The High Performance Materials Portfolio was developed with the support of many individuals. Principal Investigators, Federal Project Managers, Technology Managers, Supervisors, and National Energy Technology Laboratory site-support contractors involved with the preparation of High Performance Materials Portfolio played key roles.

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U.S. DEPARTMENT OF ENERGY

April 2018