CROSSCUTTING RESEARCH

HIGH PERFORMANCE MATERIALS PROJECT PORTFOLIO 2019

U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

DISCLAIMER

CONTENTS

INTRODUCTION

The Crosscutting Research Program advances and accelerates promising fossil energy technology by serving as a bridge between basic and applied research. The program intersects the core capabilities of the National Energy Technology Laboratory (NETL) and combines researchers' expertise to address the nation's energy priorities. Its primary agenda is to serve as a space which matures and enables commercialization of novel technologies to enhance new and existing coal-fired power plants and reduce water consumption. As the research matures it benefits other Department of Energy (DOE) Office of Fossil Energy (FE) program areas such as those under Advanced Energy Systems. Due to the broad applicability of the Crosscutting portfolio, technologies tend to generate spillover benefits in other sectors, including gas-based power generation, oil and gas infrastructure, and aviation (both commercial and military).

On behalf of FE, NETL facilitates crosscutting research and development (R&D) through collaboration with other government agencies, world-renowned national labs, start-up and established businesses and academic institutions. Through collaboration, the program advances capabilities that accelerate progress toward enabling the next generation of fossil energy. These efforts address both known existing challenges to the coal fleet as well as developing key technologies to benefit the future of coal power. Enhancements to the fleet include improvements to plant efficiency, advancements addressing the challenges of load following and cyber intrusions, and developments in affordable, scalable technical solutions. The program invests in these enhancements to secure flexible, reliable coal power for future generations.

The Crosscutting Research Program sponsors two of the longest-running university training programs, preparing the next generation of scientists and engineers to meet future energy challenges. These are the University Coal Research (UCR) program and the Historically Black Colleges and Universities and Other Minority-Serving Institutions (HBCU-OMI) program. By training at the university level with students excited about technologies on the horizon, several key technology trends will become embedded in coal plants of the future including: advanced manufacturing, cybersecurity, smart data analytics and high-performance computing.

The activities within the five primary research areas target enhanced fossil energy systems with the goal of creating transformational technology, improving plant efficiency, reducing water consumption and reducing costs. To generate transformational technology, the program connects water, sensors, computational simulation, workforce development and materials under a single umbrella.

In combination these investments in innovation, informed by private sector stakeholders, enable more comprehensive risk assessment and techno-economic analysis, increase the resiliency of our Nation's fossil energy infrastructure and enable the adoption of cutting-edge data technologies for plant owners and operators.

The Crosscutting Research portfolio of programs fosters the development of innovative power systems by conducting research in the following key technology areas:

Sensors and Controls provides pivotal insights into optimizing plant performance, reliability and availability while utilizing and furthering technological megatrends such as advanced manufacturing processes and Industry 4.0 principles.

Sensor research is investigating a range of advanced manufacturing techniques to determine the feasibility of embedding sensors, capable of operation in extreme environments and outfitted with condition-based monitoring algorithms, into turbine blades, boiler walls, piping, and tubing to predict component failure, anticipate maintenance needs and reduce plant downtime.

Controls research is advancing the accuracy of artificial and distributed intelligence systems for process control, automation, and fault detection. The ability to monitor key plant parameters and align results in real-time with self-organizing information networks will enable decision-makers to improve the operational efficiency during challenging transient conditions, increase plant availability and dispatch, tighten cybersecurity and environmental control, and improve plant revenue profiles.

This program is exploring advances within, and the integration of technologies across, three primary platforms: Advanced Sensors, Distributed Intelligent Controls, and Cybersecurity.

High Performance Materials focuses on material discovery and development that will lower the cost and improve the performance of fossil-based power-generation systems.

Materials of interest are those that enable components and equipment to perform in the high-temperature, high-pressure, corrosive environments of an advanced energy system with specific emphasis on durability, availability and cost both within and across each of four primary platforms: Computational Materials Design, Advanced Structural Materials, Functional Materials for Process Performance, and Advanced Manufacturing.

Modeling, Simulation and Analysis applies simulation and modeling capabilities to the full range of maturities and technologies essential to plant operation, from fundamental energy science in reactive and multiphase flows to full-scale virtual and interactive plant performance.

This program supports the development and application of new and innovative physics- and chemistry-based models and computational tools at multiple scales (atomistic, device, process, grid, and market) and investigates the potential positive impact these tools may have in overcoming complexities that confound today's experimental scientists and influencing the discovery of a new generation of advanced fossil-fuel technologies.

Analysis and visualization tools are manipulated to gain scientific insights into complex, noisy, high-dimensional, and high-volume datasets. The information generated is then collected, processed and used to inform research that combines theory, computational modeling, advanced optimization, experiments, and industrial input with a focus in three main platforms: Multiphase Flow Science, Advanced Process Simulation, and Innovative Concept Analysis.

Water Management aims to reduce the amount of freshwater used by fossil-fueled power plants and to minimize the potential impacts of plant operations on water quality.

The vision for this program is to develop a 21st century America that can count on our Nation's abundant, sustainable fossil energy and water resources to achieve the flexibility, efficiency, reliability, and environmental quality essential to our continued economic health and national security.

Thermoelectric power generation accounts for more than 40 percent of freshwater withdrawals (143 billion gallons of water per day) and more than 3 percent of freshwater consumption (4 billion gallons per day) in the United States. As the cost associated with water consumption increases, so will the cost of water treatment, recovery, and reuse.

The Water Management Program addresses the competing needs for water consumption through research in three dynamic platforms: Increasing Water Efficiency and Reuse, Treatment of Alternative Sources of Water, and Energy Water Analysis.

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 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. 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 °C.
- Develop advanced metallic and ceramic coatings, including nanomaterials, to provide thermal barrier protection for turbine blades, combustor components, and tubing.
- Develop validated computational models capable of simulating and predicting performance of materials in various types of transformational power 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 describes the technology, the program goals, and overall benefits.

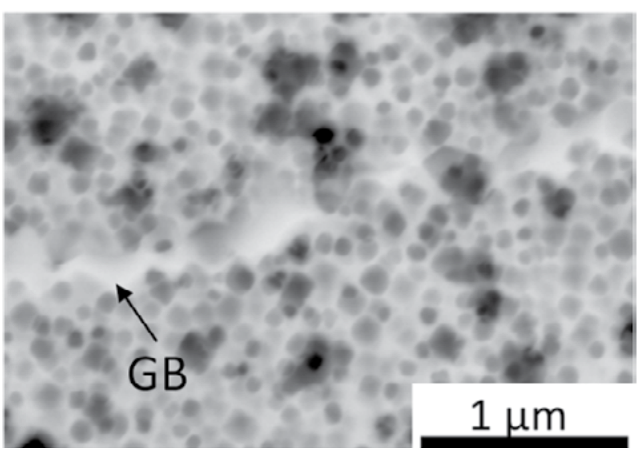
ADVANCED MANUFACTURING

Additive Manufacturing of High Gamma Prime Alloys

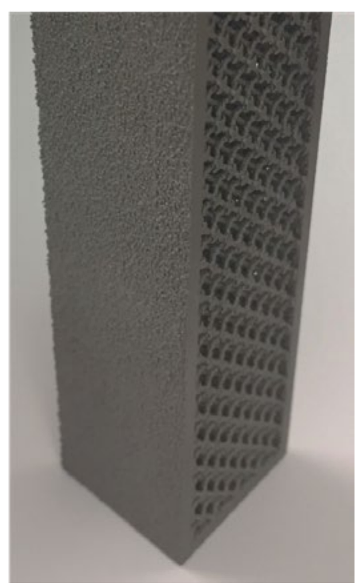
Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA127
Project Duration	9/1/2017 – 9/30/2019
Total Project Value	$ 424,000
Collaborator	Siemens
Technology Area	Plant Optimization Technologies

NETL is partnering with Oak Ridge National Laboratory (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). 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 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 Haynes 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.



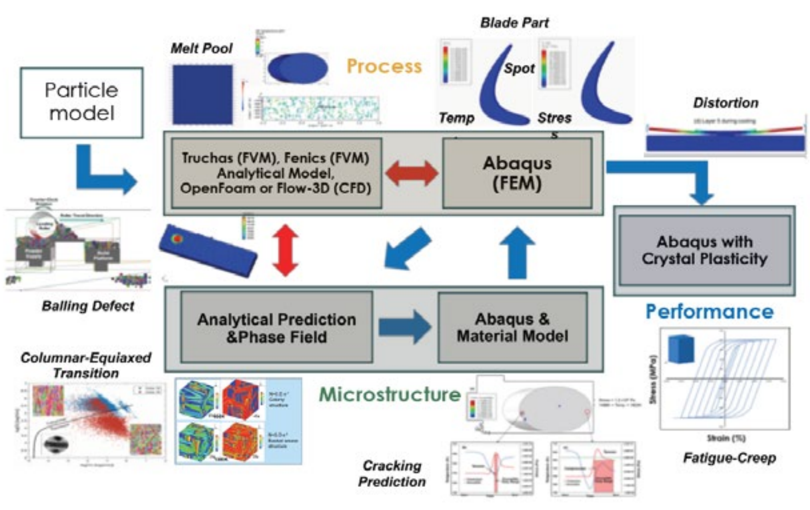
Example of a complex Haynes 282 mesh structure fabricated by electron beam melting.

Components Fabricated by Additive Manufacturing

Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA128
Project Duration	10/1/2018 – 9/30/2021
Total Project Value	$ 900,000
Collaborator	Siemens
Technology Area	Plant Optimization Technologies

The goal of this project is to develop predictive tools to correlate additive manufacturing (AM) process parameters with bulk material properties of components using machine learning algorithms. There are several key challenges currently confronting AM processes for metal-based alloys. The internal microstructures, micro-, meso- and macro- (or part-) level physical properties and performance under load are all dependent on the manufacturing process. The large number of AM processing parameters available means that AM manufacturing R&D can be very long and expensive if done without the use of process and materials modeling tools. With modeling, the various interactions and parameter sensitivities can be investigated independently from each other. For AM, where the understanding of the effects of feedstock properties, deposition rates, thermal history, cooling rates, phase transformation, defect formation, and residual stress are still in an early phase, the framework to accurately predict the part properties is not well established.

Various physics-based models will be developed to describe all steps of the AM process, allowing the determination of the alloy microstructure and mechanical properties based on the AM process parameters. A machine learning approach will also be investigated to enable rapid qualification of high-temperature structural alloys with increased additive manufacturing process reliability, which will enable design flexibility for full utilization of additive manufacturing. Collaboration between ORNL and Siemens will provide a unique opportunity of developing a simulation process that connects the process parameters through modeling to part microstructure and bulk mechanical properties and validate the process through test data on CM 247 and Haynes 282 alloys.



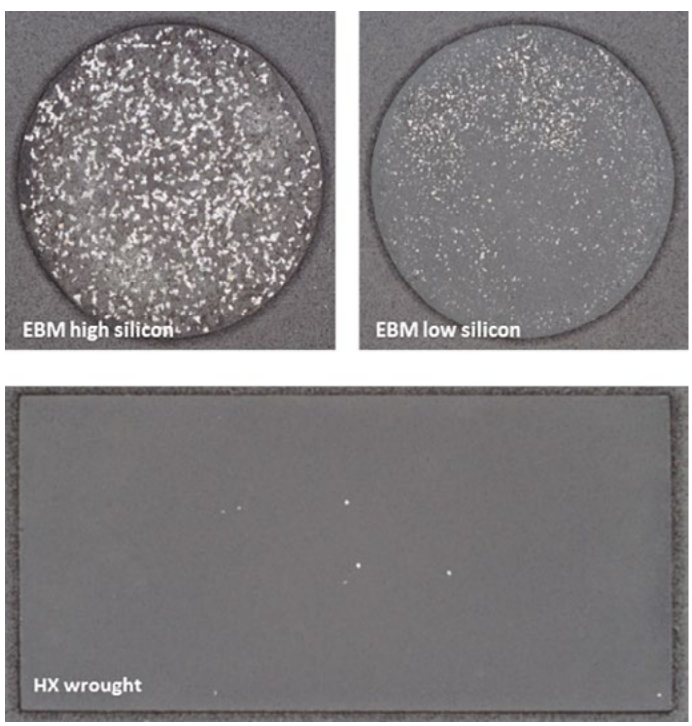
Model structure for prediction of AM process-microstructure-property correlations.

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

Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA119
Project Duration	9/1/2015 – 9/30/2019
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-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.

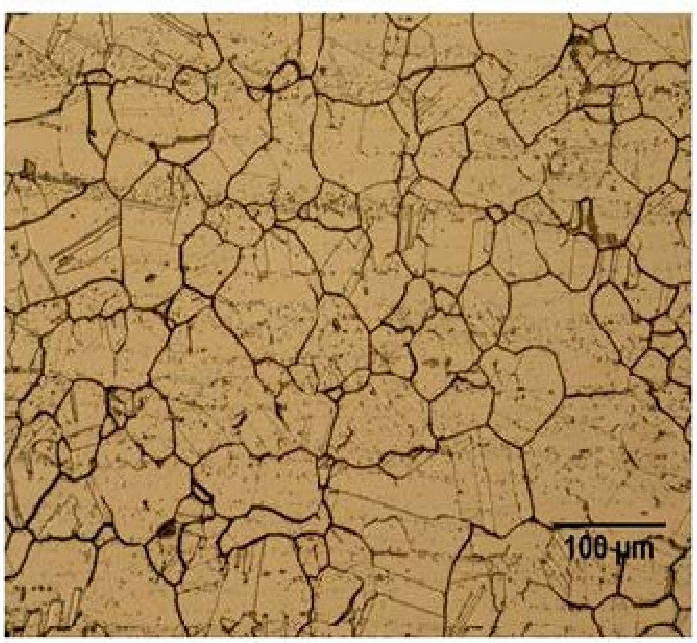


No spallation for wrought HX 4x100 hours at 950 °C.

Integrated Process Improvement Using Laser and Friction Stir Processing for Nickel Alloys Used in Fossil Energy Power Plant Applications

Performer	**Pacific Northwest National Laboratory**
Award Number	FWP-71843
Project Duration	10/1/2018 – 9/30/2021
Total Project Value	$ 1,120,000
Technology Area	Plant Optimization Technologies

The goal of this project is to determine the advantages of laser and friction stir processes when applied to the processing of nickel-based alloys used in extreme operating environments found in fossil energy power systems. This project will investigate and demonstrate an integrated approach using both laser processing (LP) and friction stir welding and processing (FSW/P) to join, repair, and return to service nickel alloy castings and wrought fabrications such as hot gas path components in gas turbine applications. The proposed integrated approach will use laser cleaning followed by friction stir welding, which may be a low-cost and robust way to increase the service life of these alloys and components used in fossil energy applications (e.g., gas and steam turbines, AUSC and sCO_2 heat exchangers).



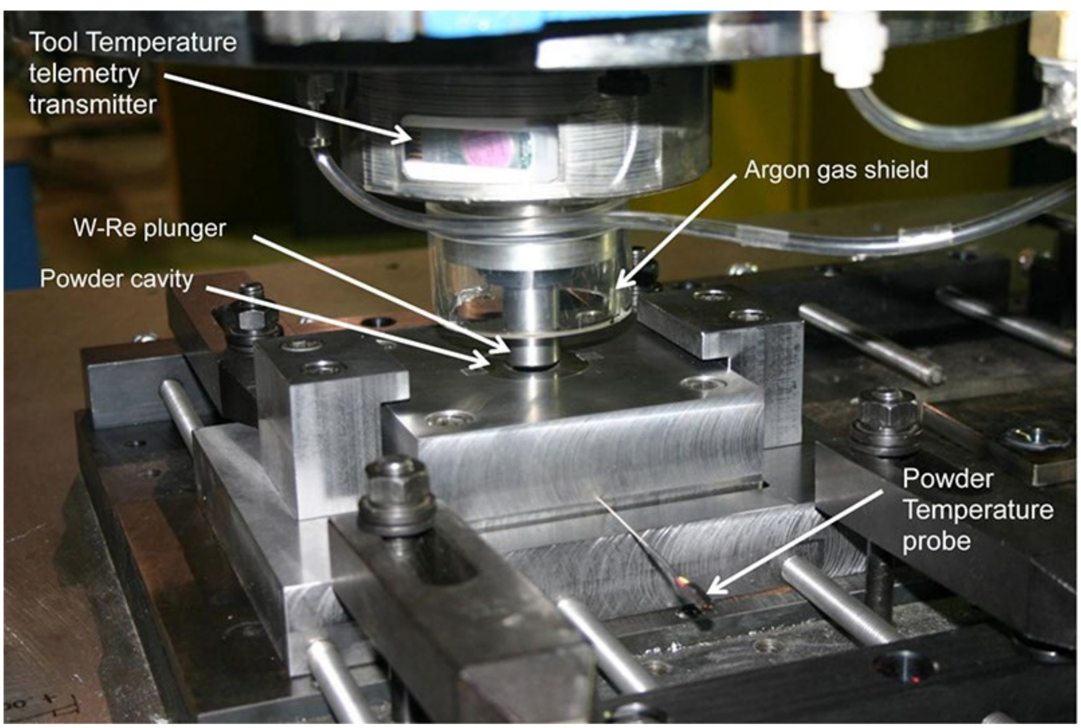
Haynes 282 microstructure comparison of base material (left) and FSW weld nugget (right).

Low Cost Fabrication of ODS Materials

Performer	**Pacific Northwest National Laboratory**
Award Number	FWP-60098
Project Duration	10/1/2010 – 9/30/2019
Total Project Value	$ 735,000
Technology Area	Plant Optimization Technologies

NETL is partnering with Pacific Northwest National Laboratory (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
Award Number	FWP-66059
Project Duration	10/1/2014 – 9/30/2019
Total Project Value	$ 1,075,000
Technology Area	Plant Optimization Technologies

NETL is partnering with Pacific Northwest National Laboratory (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.

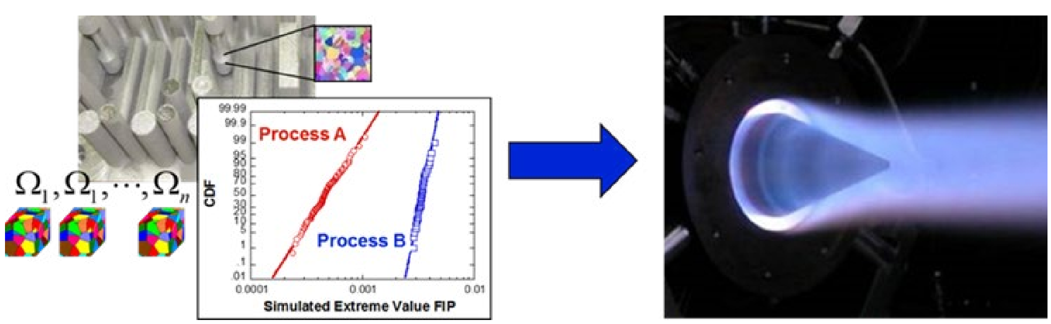
Flat plate friction stir welds in HSLA65 plate.

Digital Twin Model for Advanced Manufacture of a Rotating Detonation Engine Injector

Performer	**Southwest Research Institute**
Award Number	FE0031644
Project Duration	10/1/2018 – 9/30/2020
Total Project Value	$ 937,371
Collaborators	Aerojet Rocketdyne, Inc.; Georgia Tech Research Corporation
Technology Area	Coal Utilization Science

Southwest Research Institute (SwRI) will use a digital twin material model (DTMM) to apply advanced manufacturing techniques to advance rotating detonation engine (RDE) injector design. The project will develop both a digital twin model of the injector manufacturing process and an injector that performs in an RDE combustor with a significant reduction in flow loss. This will be accomplished through several subordinate objectives: design of a novel RDE injector that allows for fuel and oxidizer flows to be optimized in ways not possible with conventional manufacturing; comprehensive design of experiments (DofE) focusing on contributing factors that trigger high-cycle fatigue; development of a parametric material model based on actual test coupons from the advanced manufacturing process that allows prediction of mechanical strength properties; and manufacture, test, and post-test destructive evaluation of an RDE injector exposed to a significant high-cycle fatigue environment. SwRI is responsible for the material model DofE, producing a portion of the material samples; performing the detailed RDE injector design; performance testing of the RDE injector; and post-test analysis of the injector component. Aerojet Rocketdyne will support the application of this work to the existing RDE; review the DofE for material samples; produce many of the material samples; support the conceptual design of the new RDE injector; manufacture the RDE injector prototypes for testing; and support RDE injector testing, including data capture and post-processing. Georgia Institute of Technology will provide the material model development and application to the design of the RDE injector; review the DofE for completeness; process material samples to extract physical and microstructure qualities; advance the process parameter to microstructure linkage; develop the microstructure to fatigue resistance linkage; and support the injector design analysis with process parameter optimization.

The development, implementation, and validation of tools for predicting and verifying microstructural properties, strength, residual stress, and dimensional build characteristics has extremely high relevance for high-temperature high-strength applications that may benefit from additively manufactured parts. Development of a digital twin model of an RDE injector manufacturing process, and an injector that performs in a RDE combustor with a significant reduction in flow loss, will allow the RDE injector to transition to the industrial application of fossil based power generation.



Modeling of additively manufactured parts leading to low-loss additively manufactured RDE injector.

ADVANCED STRUCTURAL MATERIALS

eXtremeMAT: Extreme Environment Materials

Performer	Ames National Laboratory	Idaho National Laboratory	Lawrence Livermore National Laboratory	Los Alamos National Laboratory	National Energy Technology Laboratory	Oak Ridge National Laboratory	Pacific Northwest National Laboratory
Award Number	FWP-AL-17-510-091	FWP-B000-17016	FWP-FEW0234 / FWP-FEW0252	FWP-FE-850-17-FY17	FWP-1022433	FWP-FEAA134	FWP-71133
Project Duration	9/1/2017 – 9/30/2019	9/1/2017 – 9/30/2019	9/1/2017 – 9/30/2019	9/1/2017 – 9/30/2019	9/1/2017 – 9/30/2019	9/1/2017 – 9/30/2019	9/1/2017 – 9/30/2019
Total Project Value	$ 505,000	$ 454,000	$ 311,000	$ 1,180,000	$ 439,000	$ 696,000	$ 629,000
Total Project Value (All)	$ 4,214,000						
Technology Area	Coal Utilization Science						

Affordable, durable, cost effective, heat-resistant alloys are necessary for improving the existing fleet of fossil energy power plants, and enabling advanced fossil energy systems, such as advanced ultrasupercritical Rankine cycles and supercritical carbon dioxide (sCO_2) power cycles. Accelerating the development of improved steels, superalloys, and other advanced alloys is of paramount importance in deploying materials solutions to meet the challenges with fossil energy power generation.

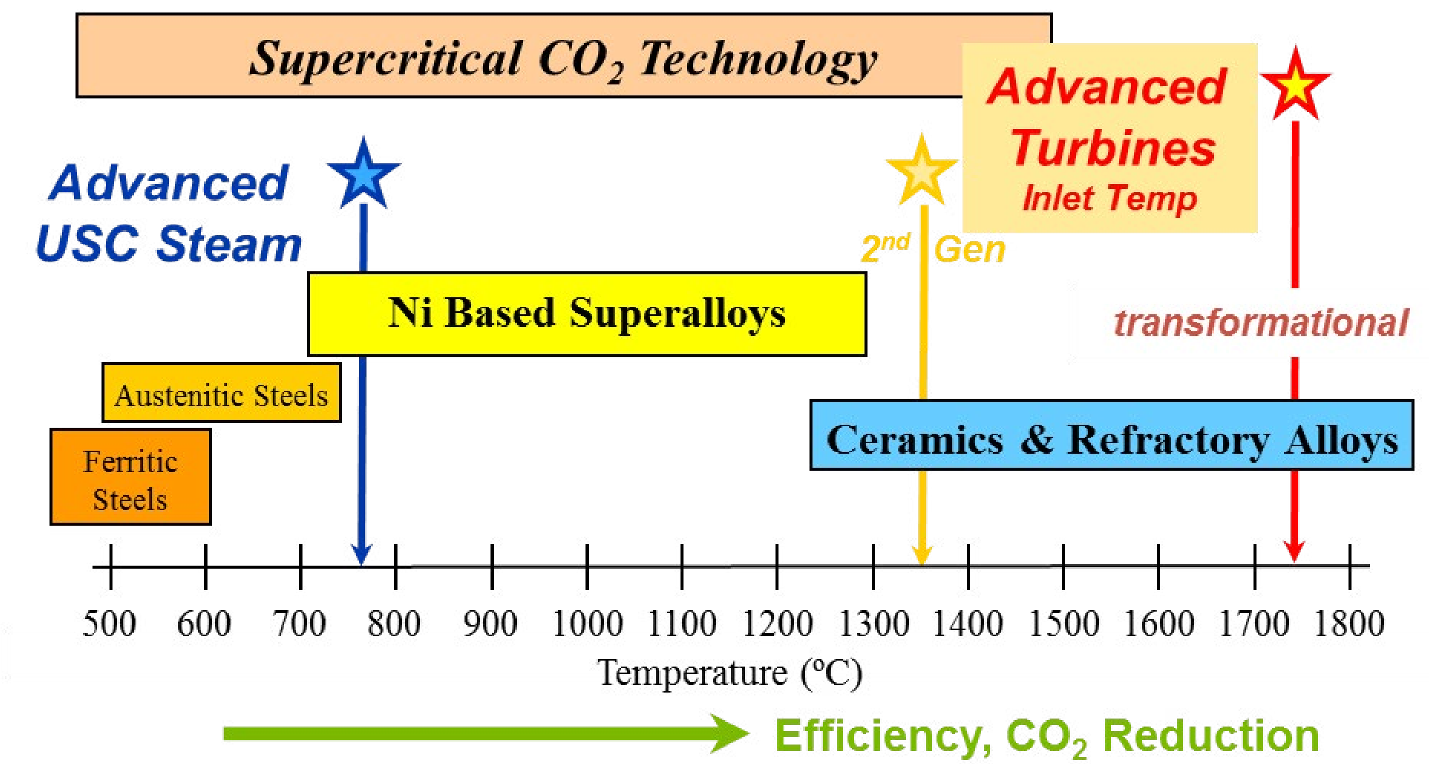
eXtremeMAT brings together seven of the leading national laboratories to harness the unparalleled breadth of unique capabilities across the DOE complex associated with materials design, high-performance computing power, advanced manufacturing, in-situ characterization, and performance assessment at condition into an integrated, mission-focused team, focused on:

- Developing a suite of improved heat resistant alloys for fossil energy components in existing and future power plants
- Predicting long-term materials performance in existing and future fossil energy power cycles

The objective of eXtremeMAT is to demonstrate how state-of-the-art computational materials modeling and cutting-edge experimental tools can accelerate development and deployment of new heat-resistant alloys for fossil energy applications. In addition, materials modeling and life prediction and the models developed therein can be used to assess the current and remaining life integrity of heat-resistant alloys used in existing plants. It may also be possible to improve the performance envelope of current-generation fossil energy alloys by understanding the relationship between manufacturing, microstructural stability, and mechanical behavior.

Initially, the effort will target enabling sCO_2 technologies through the development of high yield strength, high-temperature austenitic stainless steel alloys. Although nickel (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 lower-cost alloys, thereby reducing the amount and cost of nickel 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 degrees Celsius, while maintaining low costs 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 percent chromium steels and higher-performance alloys such as Ni-based or high-entropy alloys.

In the near term, the project team is working to identify promising candidates for new low-cost iron-based alloys that would perform well in an sCO_2 environment. In the long term, the team aims 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.



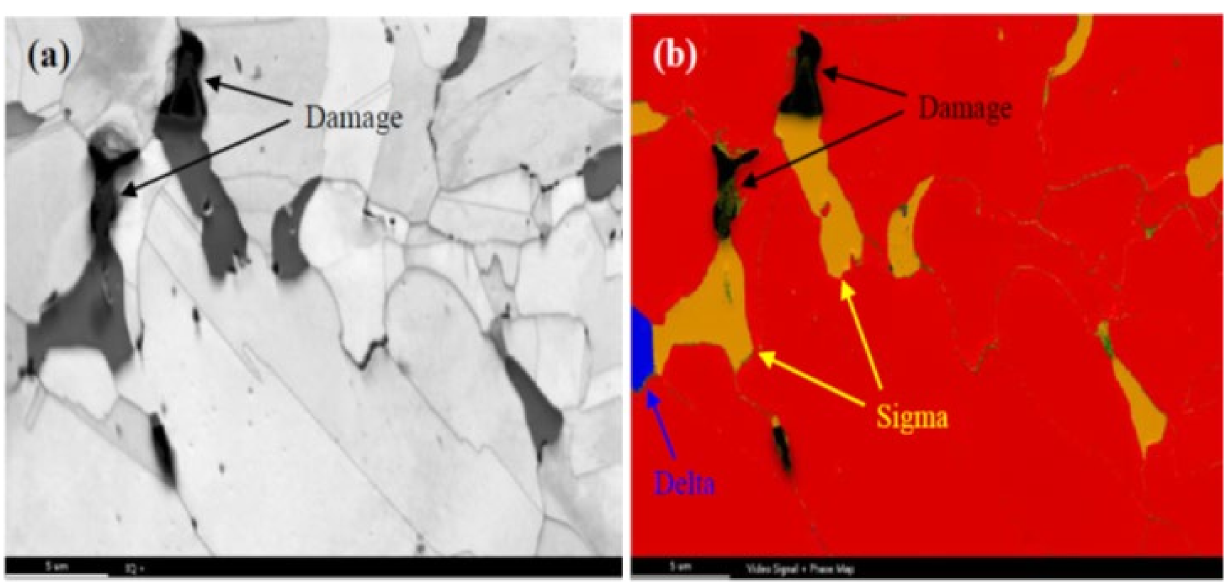
Extreme environment materials for advanced fossil energy power generation.

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

Performer	**Electric Power Research Institute, Inc.**
Award Number	FE0031562
Project Duration	1/25/2018 – 1/24/2021
Total Project Value	$ 2,500,000
Technology Area	Advanced Combustion Systems

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.



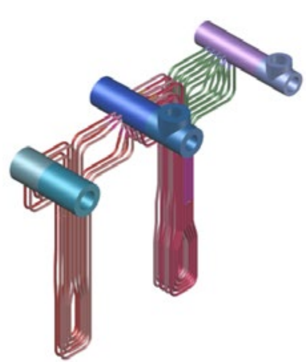
(a) Scanning electron microscope image and (b) corresponding electron backscatter diffraction phase map showing creep damage associated with sigma phase in 374H.

Advanced Ultra-Supercritical Component Testing

Performer	**Energy Industries of Ohio, Inc.**
Award Number	FE0025064
Project Duration	11/1/2015 – 9/30/2021
Total Project Value	$ 26,750,822
Collaborators	AECOM; Alstom Power, Inc.; Electric Power Research Institute, Inc.; GE Power and Water; MetalTek International; Riley Power; Special Metals; Thermal Engineering; Youngstown Thermal
Technology Area	Plant Optimization Technologies

The National Energy Technology Laboratory is partnering with Energy Industries of Ohio, Inc. to fabricate commercial-scale nickel superalloy components and sub-assemblies that would be needed in a coal-fired power plant of approximately 800 megawatts generation capacity (MWe) operating at a steam temperature of 760 degrees Celsius (1400 degrees Fahrenheit) and steam pressure of at least 238 bar (3500 pounds per square inch absolute). The original scope of work included operational testing of a small prototype-scale steam turbine and advanced ultrasupercritical (AUSC) superheater, but it was determined that this is not required. The project will (1) procure the AUSC materials that will be fabricated into AUSC components and sub-assemblies, (2) fabricate AUSC boiler and superheater components and sub-assemblies, (3) fabricate a cast nickel superalloy steam turbine nozzle carrier casing (Haynes 282), (4) fabricate forged nickel superalloy components for an AUSC steam turbine (Haynes 282) and for an AUSC main and reheat steam piping system (Inconel 740), (5) conduct testing and obtain American Society of Mechanical Engineers code stamp approval for nickel superalloy pressure relief valve designs that would be used in AUSC power plants up to approximately 800 MWe, and (6) develop a matrix for future laboratory-scale mechanical testing and metallurgical examination of the fabricated components.

The expected benefits of the project will be (1) the development of a domestic supply chain for fabricating nickel superalloy and other AUSC power plant components, (2) validation of advanced design and life prediction methods for AUSC components that are made from nickel superalloys and other advanced creep resistant alloys in both steady state and cycling operating modes, (3) validation of the ability to design nickel superalloy and other AUSC components for operating life of least 30 years, (4) validation through design and fabrication that AUSC components can be designed and built for reliable operation under both steady-state and varying load operating conditions, and (5) development and validation of fabrication, installation and repair methods for cast and forged nickel superalloy AUSC power plant components and sub-assemblies.



AUSC superheater/reheater assembly.

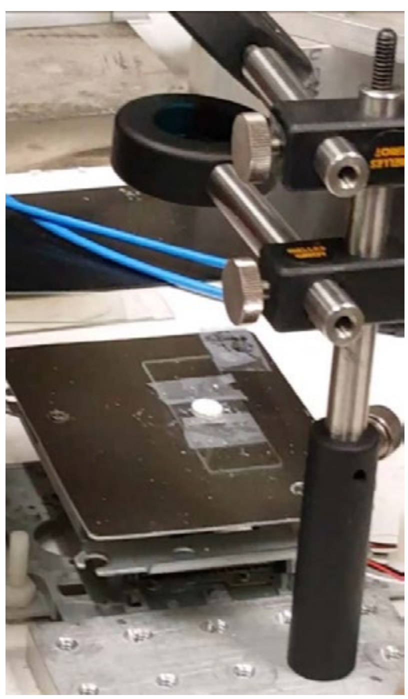
Nozzle carrier casting.

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

Performer	**Florida International University**
Award Number	FE0026325
Project Duration	10/1/2015 – 9/30/2019
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 magnetohydrodynamic (MHD) direct power extraction 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 required during the materials sintering process, resulting in less costly high-temperature ceramic materials.



Green body formation via laser cutting.

Advanced Alloy Development

Performer	**National Energy Technology Laboratory**
Award Number	FWP-1022406
Project Duration	1/1/2017 – 3/31/2019
Total Project Value	$ 6,130,000
Technology Area	Plant Optimization Technologies

NETL's Research and Innovation Center's Advanced Alloy Development Field Work Proposal (FWP) is focused on developing high-performance materials to improve efficiencies in the existing fleet and enable advanced fossil energy systems. NETL uses an integrated materials engineering approach that incorporates computational alloy design with best-practice manufacturing (modified as needed to achieve microstructure and performance objectives) with focused performance evaluation and characterization. Research is 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:

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.

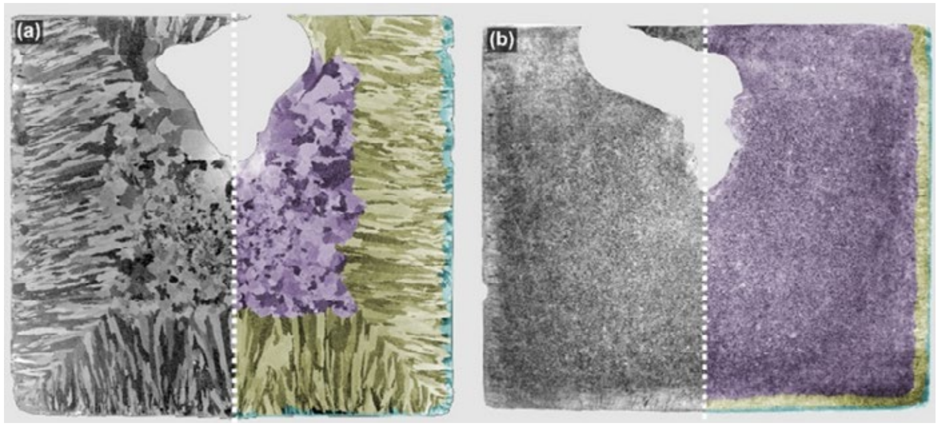
Computational Design and Simulation—Use computational materials modes, multi-scale characterization simulations of microstructural features, and cutting-edge data analytics to guide and accelerate alloy design and manufacturing development.

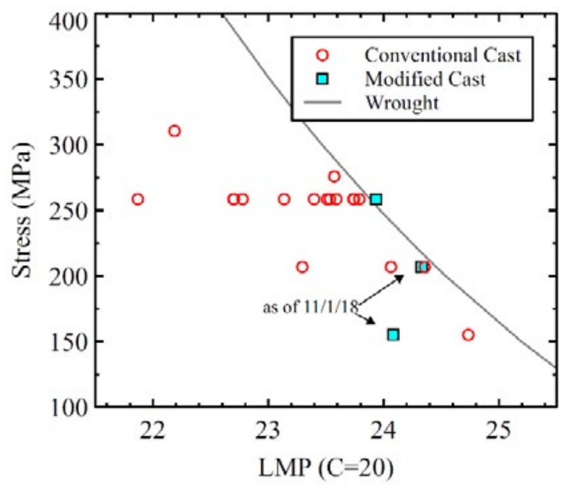
Processes, Manufacturing, and Properties—Develop and demonstrate at pilot industrial scales improved manufacturing processes to produce advanced alloys with improved service life performance.

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.

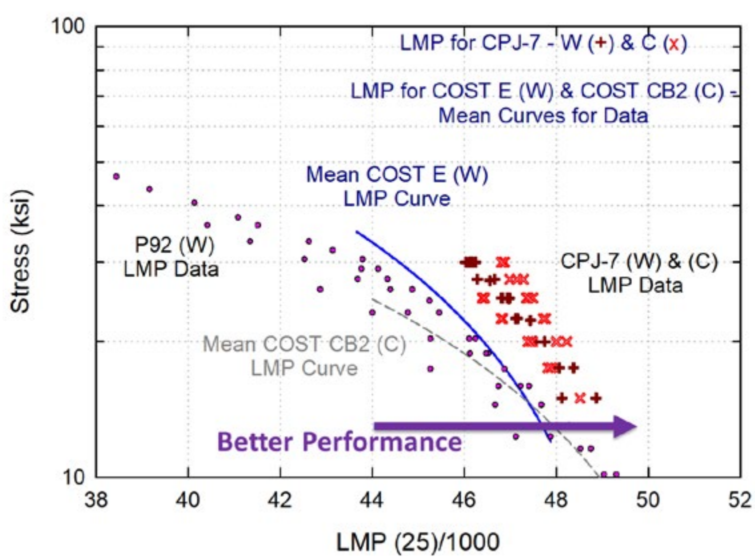
Materials for sCO_2 Power Cycles: Materials and Manufacturing Issues Associated with Heat Exchangers for sCO_2 Power Cycles—Assess materials selection and joining processes for compact heat exchanger designs to (1) reduce equipment size, and (2) enhance heat transfer between the high-temperature and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





Cast Version of Alloy 740. A modified casting route was developed that leads to a more homogeneous grain size distribution throughout the casting (b compared to a) and better properties. Creep testing is on-going, but results indicate that the modified cast materials behave in a similar manner to the wrought material.



Creep behavior NETL's CPJ-7 compared to other advanced Fe-9Cr streels, COST E, Cost CB3 and P92. W=Wrought, C=Cast.

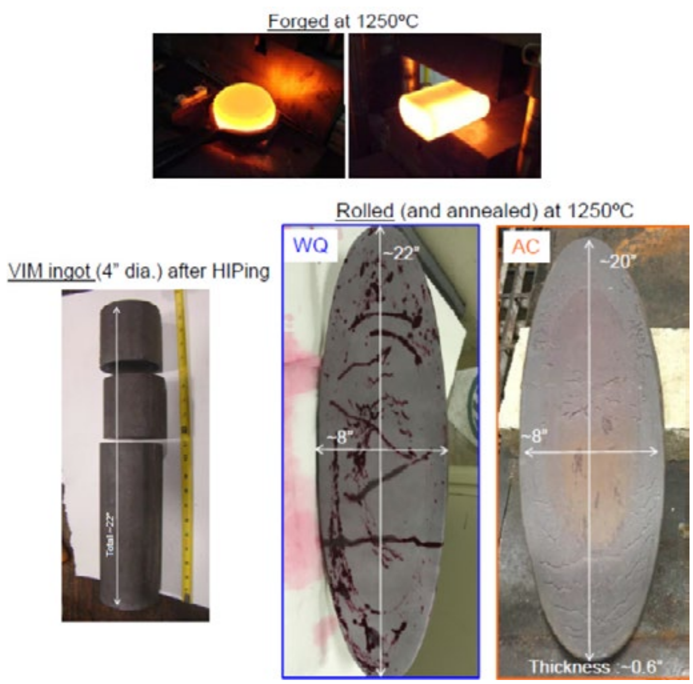
Advanced Alloy Design Concepts for High Temperature Fossil Energy Applications

Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA114
Project Duration	10/1/2013 – 9/30/2019
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**
Award Number	FWP-FEAA123
Project Duration	10/1/2015 – 9/30/2019
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 calls for continued study of 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.

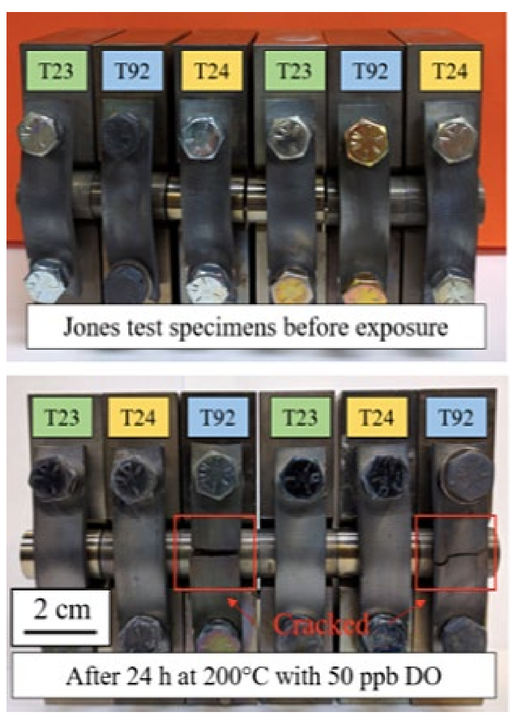
Corrosion Issues in Advanced Coal Fired Boilers

Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA116
Project Duration	10/1/2013 – 9/30/2019
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.



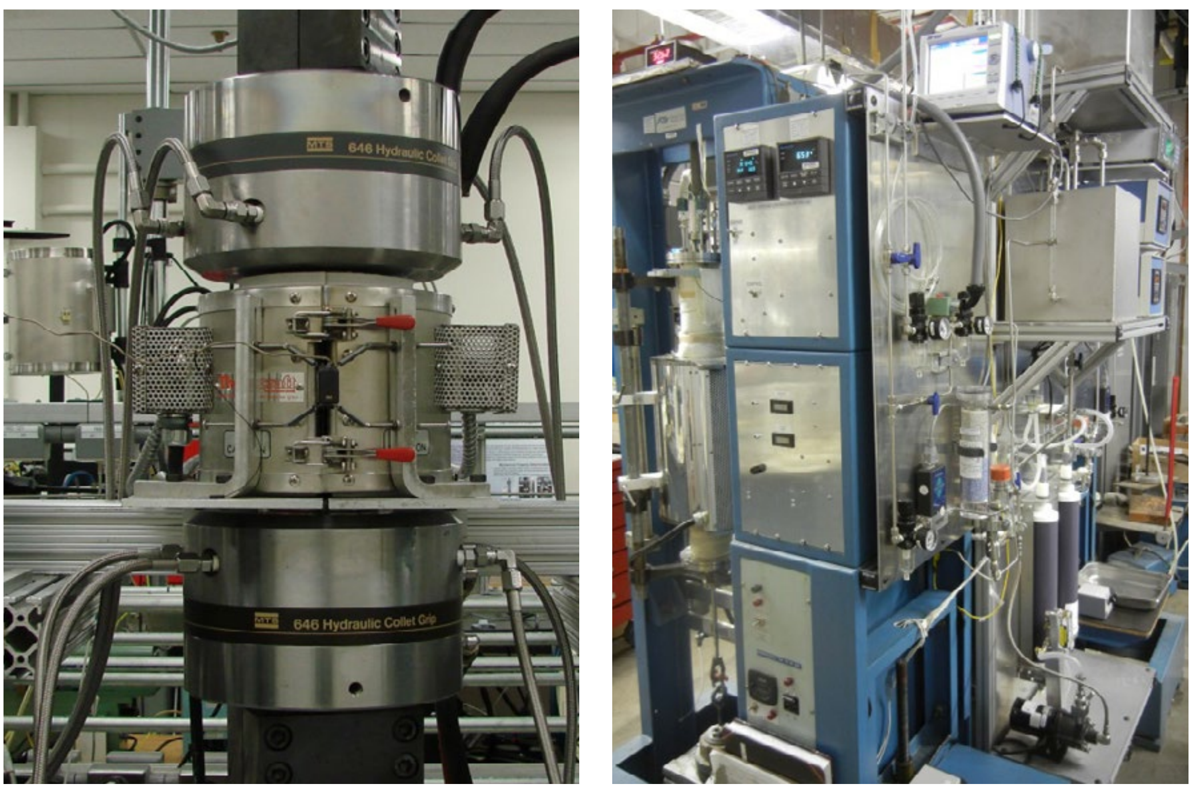
Jones tests with controlled water chemistry.

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

Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA115
Project Duration	10/1/2013 – 9/30/2019
Total Project Value	$ 1,500,000
Technology Area	Coal Utilization Science

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 flexible 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.



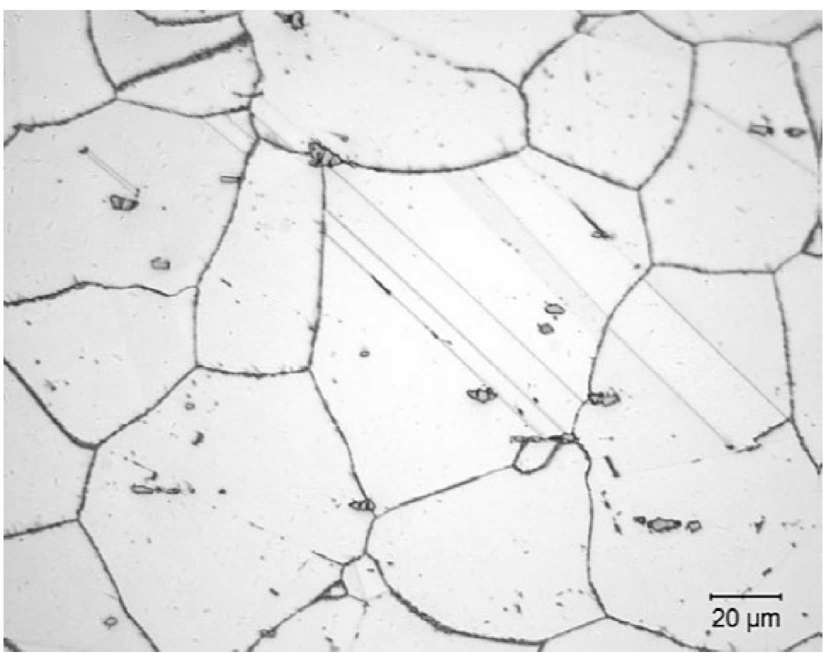
Left: Servo-hydraulic creep-fatigue machine.
Right: Thermal cyclic creep machines allowing testing in steam.

Materials Qualification and Deployment for High Efficiency Coal Fired Boilers

Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA117
Project Duration	4/1/2015 – 9/30/2019
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 hour life.



H282 microstructure in age hardened condition.

Probabilistic Life Assessment and Aged Materials Testing for Service Feedback of Gas Turbine Components

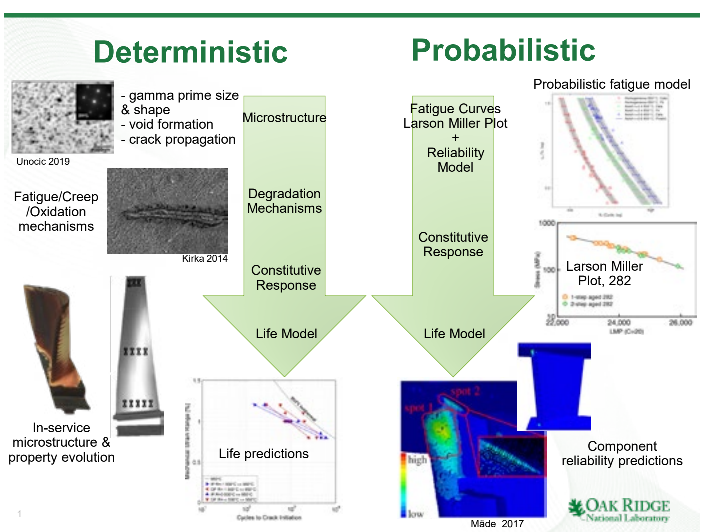
Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA137
Project Duration	10/1/2018 – 9/30/2021
Total Project Value	$ 900,000
Technology Area	Plant Optimization Technologies

The goal of this project is to improve lifetime model prediction for nickel-based superalloy power plant components. The microstructure and properties of parts exposed in the field for up to 32,000 hours will be characterized to determine the evolution of key lifetime damage parameters. Synergy between deterministic and probabilistic lifetime models will also be evaluated. Siemens will select the parts exposed in the field to be characterized and will conduct lifetime assessment using their internal probabilistic model.

Reliability of key components of the power plant such as steam or gas turbines and generators is of prime importance. Many utilities are interested in extending the life of turbine-generator components to reduce costs while maintaining safe operating conditions. During operation, these materials undergo different metallurgical degradation processes due to complex thermomechanical loadings and corrosion in aggressive environments. Assessment of the remaining life of these components and materials is essential to guide the lifetime extension of aged units through repair work, continuous inspection, and replacement of the degraded parts.

The project focus is to improve available lifetime prediction models using data obtained from nickel-based superalloy power plant components that have undergone long-term service. Technical objectives include:

- Evaluation of the complementarity between deterministic and probabilistic models for gas turbine material systems, with a focus on Haynes 282 of interest in the 600-760 °C temperature range for the AUSC program and between 800-950 °C for the gas turbine combustor section.
- Characterization of the microstructure and mechanical and thermal properties of components that have operated in power plants for 8,000 to 32,000 hours.
- Use of the microstructural characterization data to validate lifetime models based on the service history of the components.

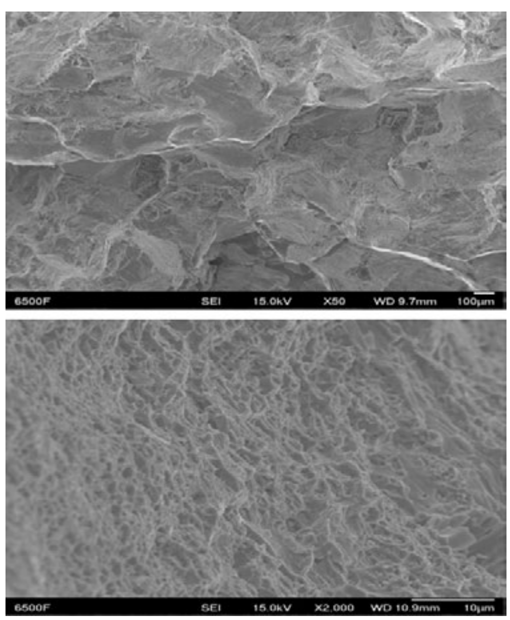


Properties of Advanced Ni-Based Alloys for A-USC Steam Turbines

Performer	Oak Ridge National Laboratory
Award Number	FWP-FEAA125
Project Duration	2/1/2016 – 9/30/2019
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)/1400 degrees Fahrenheit (°F) and 345 bar/5000 psi, 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 temperatures and applied stress conditions.



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

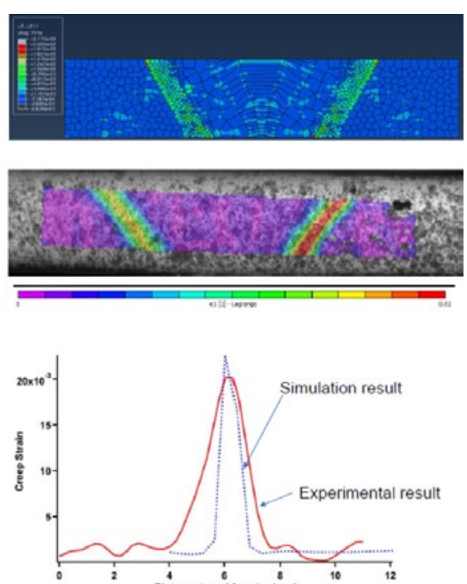
Weldability of Creep Resistant Alloys for Advanced Power Plants

Performer	**Oak Ridge National Laboratory**
Award Number	FWP-FEAA118
Project Duration	10/1/2013 – 9/30/2019
Total Project Value	$ 1,800,000
Technology Area	Coal Utilization Science

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-weld 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.



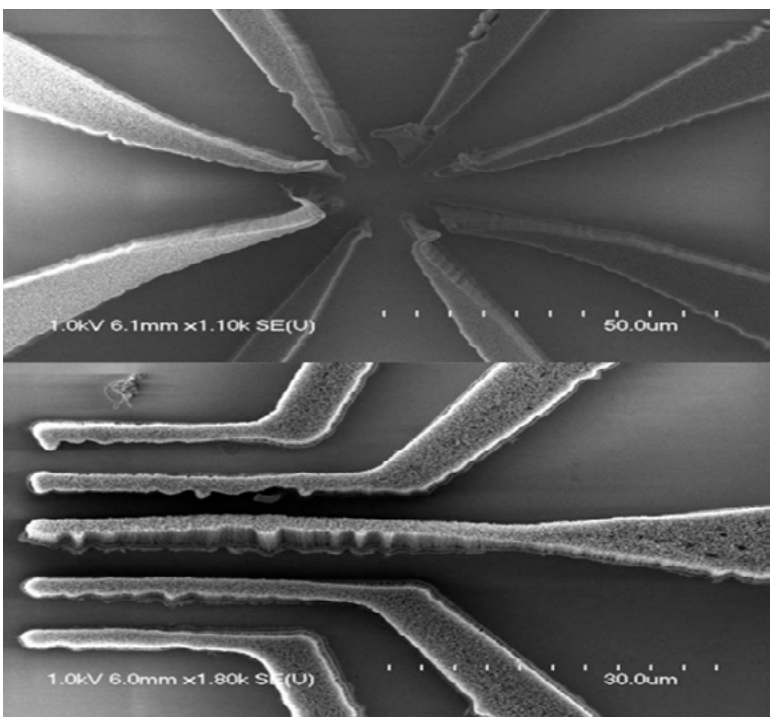
Top: Modeling result.
Middle: Experimental result.
Bottom: Simulation result shows agreement with experiments.

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

Performer	**University of Nebraska Lincoln**
Award Number	FE0023061
Project Duration	10/1/2014 – 9/30/2019
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 centimeter 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.



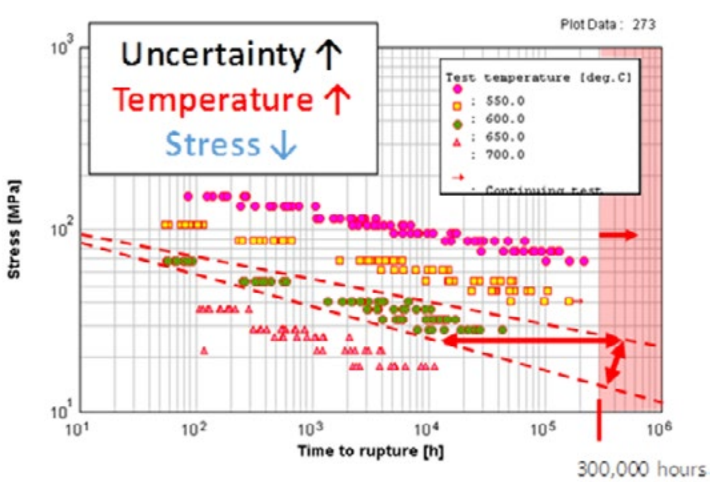
Vertically aligned CNT patterns: two potential models of the carbon dispersion within the SiC bulk.

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	9/1/2017 – 8/31/2020
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 Inconel 718 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 a 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 to which the ACTs are independent of systematic errors and calibration bias. Finally, a comprehensive standardized "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 (10^6 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.



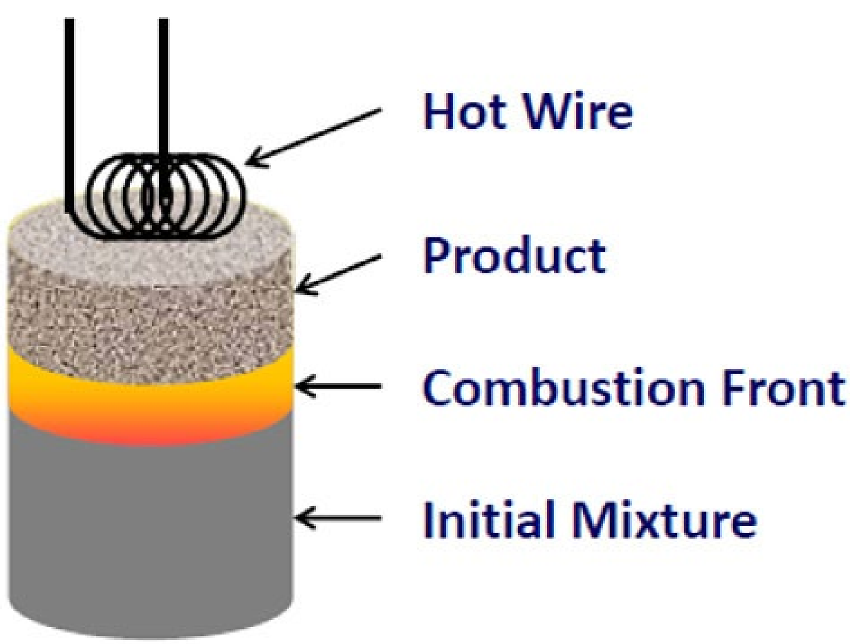
Creep-rupture of 9Cr-1Mo tube.

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	10/1/2015 – 8/31/2019
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.

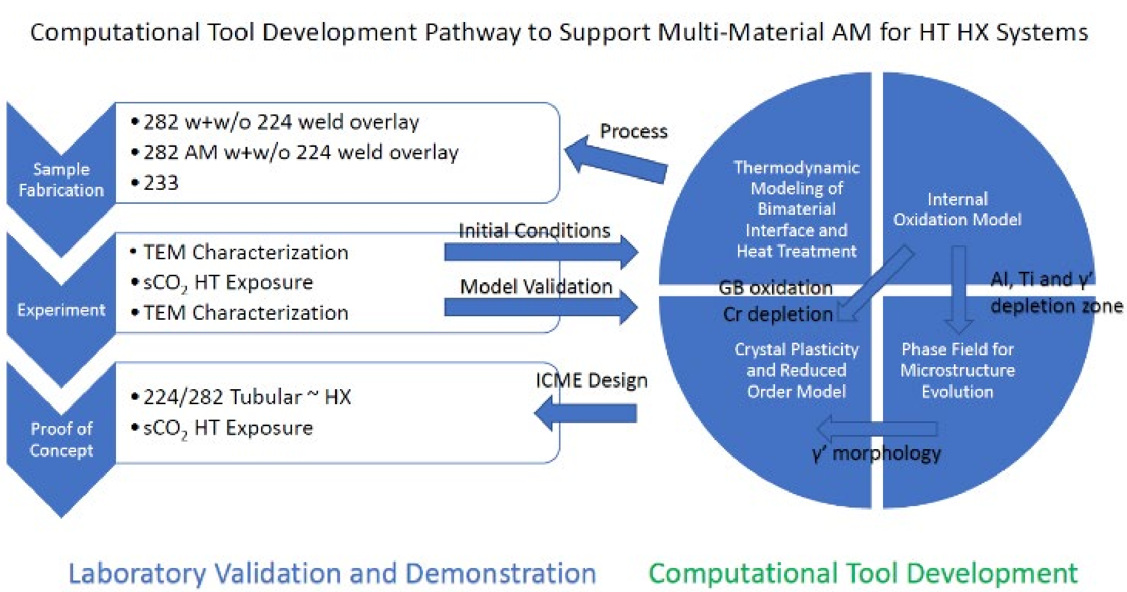
COMPUTATIONAL MATERIALS DESIGN

ICME for Advanced Manufacturing of Nickel Superalloy Heat Exchangers with High Temperature CREEP Plus Oxidation Resistance for Supercritical CO_2

Performer	**Det Norske Veritas (DNV) GL USA, Inc.**
Award Number	FE0031631
Project Duration	10/1/2018 – 9/30/2020
Total Project Value	$ 937,500
Technology Area	Coal Utilization Science

Det Norske Veritas (DNV) GL USA will develop and validate computational design and analysis tools that optimize novel material combinations for fabricating microchannel heat exchangers via additive manufacturing for supercritical CO_2 power cycle technology. Original experiments will be performed for alumina- and chromia-scale forming nickel-based superalloys made with conventional and additive manufacturing with simulated compositional grading effects. The project integrates high-temperature oxidation modeling, phase-field modeling of microstructure evolution, and creep performance using crystal plasticity modeling. The three models will be coupled according to an input-output matrix that passes information on solute depletion into microstructure models for gamma-prime (γ') re-distribution and then into the crystal plasticity models for prediction of creep rate and tensile strength reduction. The modeling work will be tightly coupled with experimental high-temperature oxidation and creep testing of advanced alloys and prototype components in supercritical CO_2.

This project could provide the fossil energy industry with new options for materials with property gradients. The integrated computational materials engineering (ICME) approach could improve pre-screening of fabrication techniques and heat treatments, which could reduce design time for materials intended for service in extreme environments.



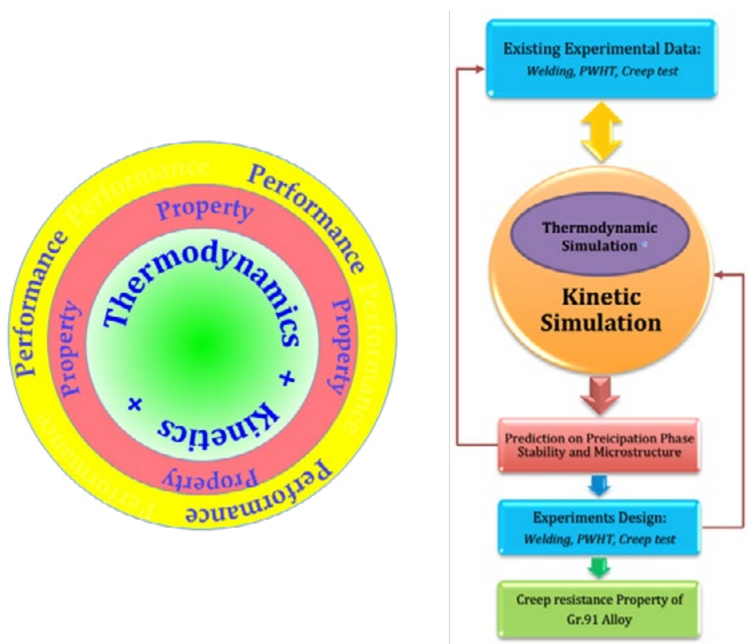
Project flow of models, experiments, and information.

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	8/1/2016 – 7/31/2019
Total Project Value	$ 250,000
Collaborator	The 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 Grade 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 Grade 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 Grade 91 alloy; develop a model that will provide an excellent match with experimental data from current and previous work on Grade 91 alloy; and predict how to improve the long-term creep resistance for the Grade 91 family of alloys.

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



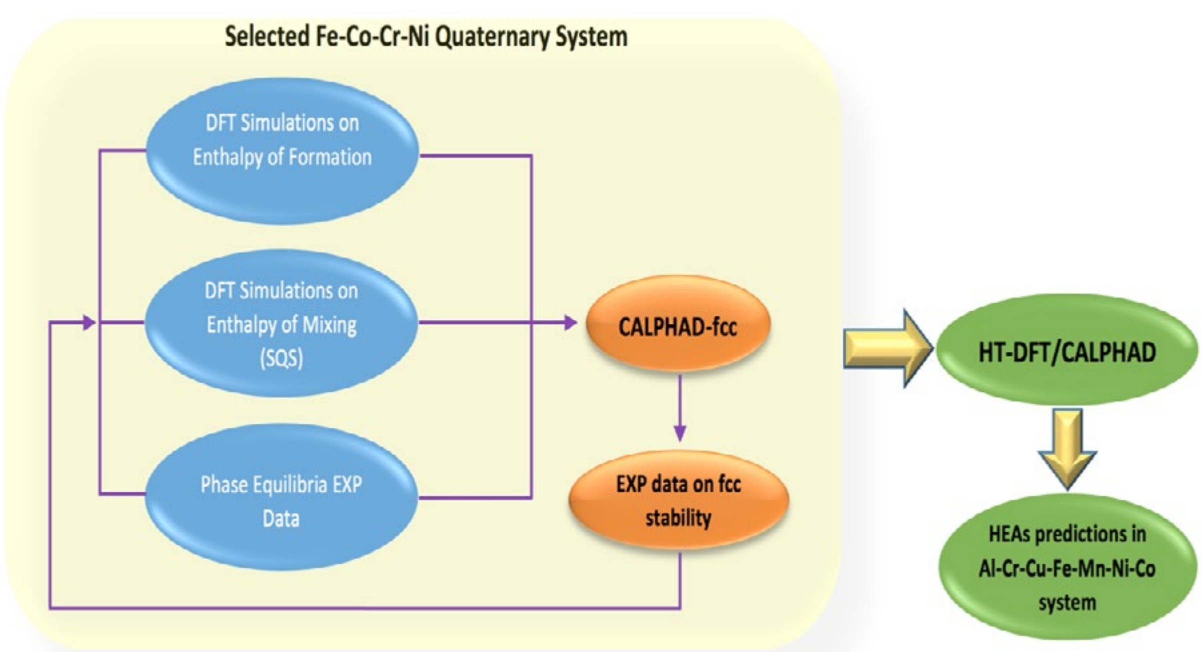
Materials design using ICME approach.

The Novel Hybrid Start-off Model of High Performance Structural Alloys Design for Fossil Energy Power Plants

Performer	Florida International University
Award Number	FE0030585
Project Duration	8/1/2017 – 7/31/2020
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.



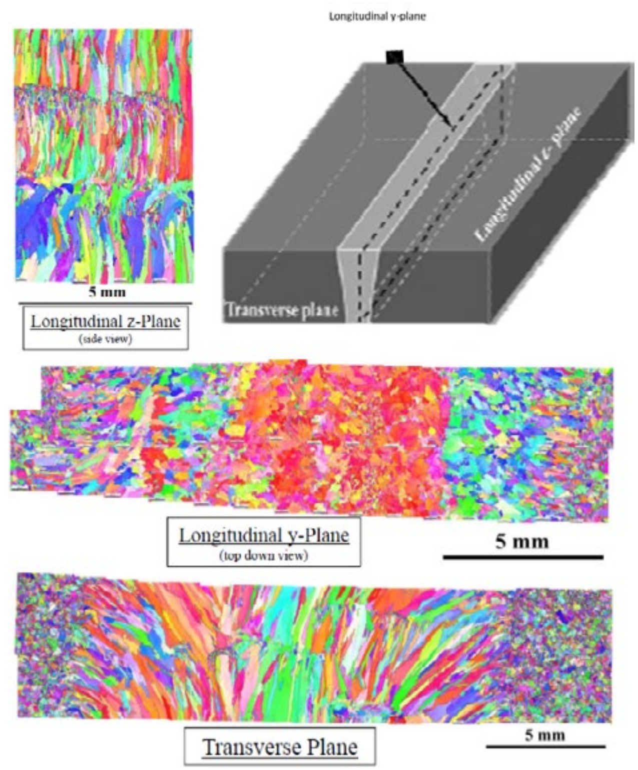
Development of the hybrid ab initio/CALPHAD approach.

Physics-based Creep Simulation of Thick Section Welds in High Temperature and Pressure Applications

Performer	**Idaho National Laboratory**
Award Number	FWP-B000-14029
Project Duration	6/1/2015 – 9/30/2019
Total Project Value	$ 955,000
Technology Area	Coal Utilization Science

Idaho National Laboratory (INL) will improve the capability to perform accurate and rapid computational modeling of the long-term mechanical behavior of nickel superalloy weldments that will be used in advanced fossil energy power cycles. An improved capability to predict the long-term behavior of weldments will allow materials scientists and structural component designers to optimize the use of advanced materials in advanced fossil energy applications. In this project INL will develop a microstructure-based creep model for nickel superalloys and add it to a computational platform, Multiphysics Object-Oriented Simulation Environment (MOOSE), that INL has developed for multi-scale simulation of the behavior of high-temperature materials in nuclear power plant applications.

This project will develop improved computational methods to predict the long-term behavior of advanced materials and structural components in fossil energy power plants that will reduce the time and expense of developing and qualifying new materials and enable a more cost-effective use of advanced materials at higher operating temperatures and pressures, which will result in higher-efficiency fossil fuel based power systems.



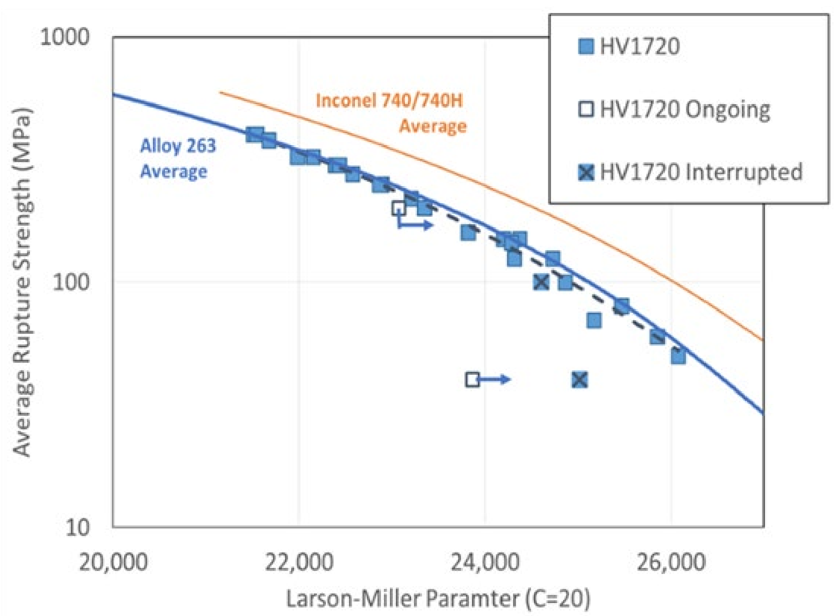
Microstructure of base metal, heat affected zone, and weld metal.

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

Performer	**Michigan Technological University**
Award Number	FE0027822
Project Duration	8/15/2016 – 8/14/2019
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 η + γ', 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.



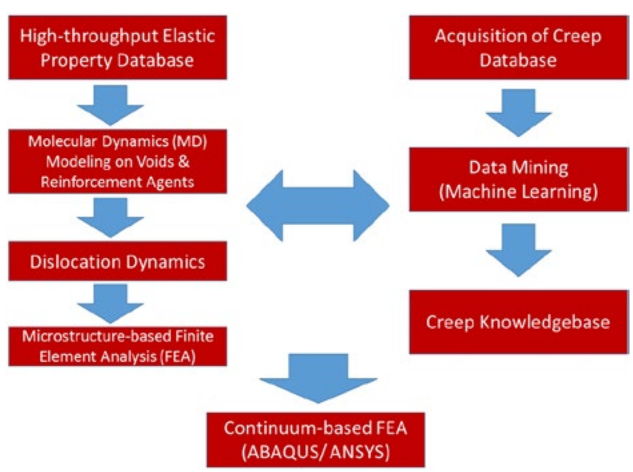
Alloy 20, Widmanstätten microstructure, creep.

Multi-modal Approach to Modeling Creep Deformation In Ni-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; University of Missouri–Kansas City
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.



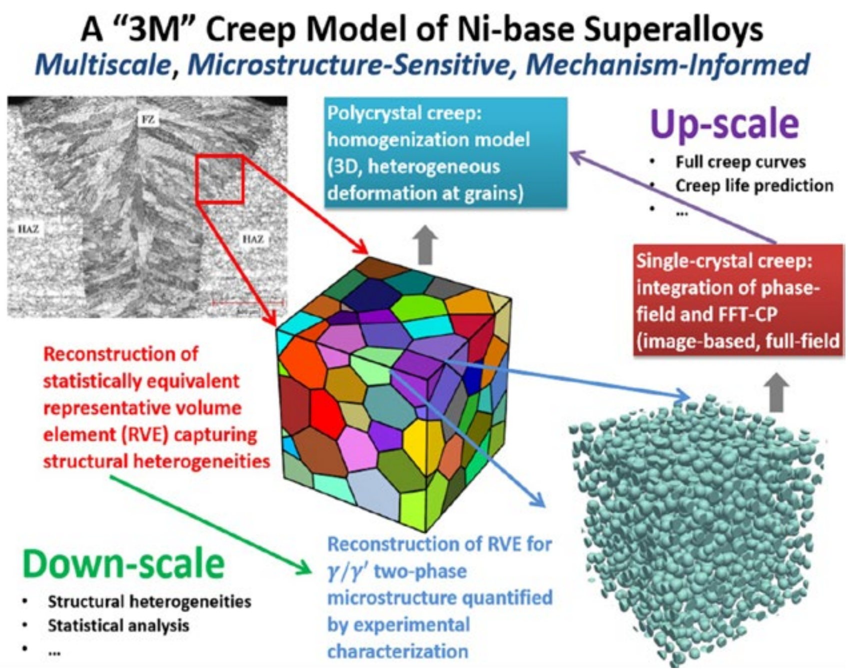
Schematics of overall multi-modal workflow of proposed new roadmap to integrate the use of experimental creep database ("top-down" approach) with multi-scale modeling ("bottom-up" approach).

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

Performer	**Ohio State University**
Award Number	FE0027776
Project Duration	9/1/2016 – 7/31/2019
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.



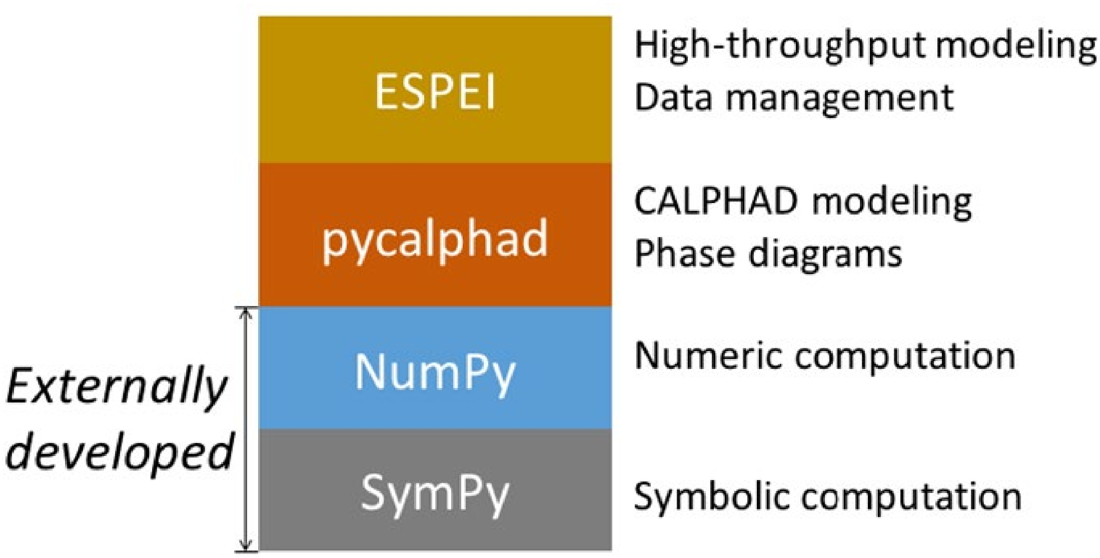
ICME approach.

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 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.

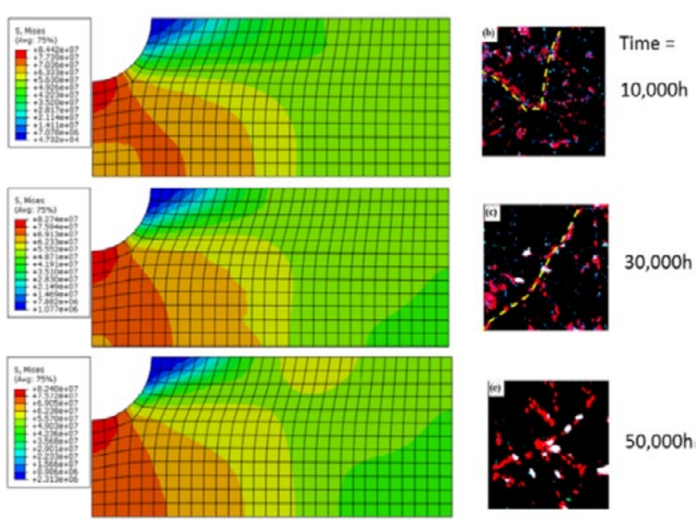


ESPEI-2.0 software stack.

Improved Models of Long-Term Creep Behavior of High Performance Structural Alloys for Existing and Advanced Technologies Fossil Energy Power Plants

Performer	**QuesTek Innovations, LLC**
Award Number	SC0015922
Project Duration	6/13/2016 – 7/30/2019
Total Project Value	$ 1,164,586
Technology Area	Plant Optimization Technologies

NETL is partnering with QuesTek Innovations LLC to develop a robust creep modeling toolkit to predict the long-term creep performance of materials for base alloys and weldments in fossil energy systems under wide thermal and mechanical conditions. Precipitation modeling using thermodynamic databases will provide fundamental quantities that will be used as inputs for upscaling strategies and methods. The goal is to establish microstructure-sensitive models that capture the different creep mechanisms observed in ferritic steels and integrate the models into QuesTek's Defense Advanced Research Projects Agency - Accelerated Insertion of Materials (DARPA-AIM) efforts to predict the variability of the creep strength as a function of the microstructure and service conditions. In the Phase I effort, the methods proposed have been demonstrated to predict creep life near 100,000 hours for P91 ferritic steels with microstructure inputs obtained from the National Institute of Material Science. In Phase II, the tools will be expanded and exercised in wider operating conditions including different temperatures and applied stresses in order to predict creep behaviors with over 300,000 hours creep life. Integration of precipitate evolution schemes into the long-term material behavior (i.e., stability of microstructure and the different phases over long periods), along with a refined uncertainty quantification of various material and process parameters, will be assessed and calibrated in Phase II. Additionally, the methodology that is developed would be applicable to alternative material systems and microstructures through additional modules that capture the relevant mechanisms of creep. Accurate and efficient quantification of material properties for advanced ultrasupercritical (AUSC) boilers will directly enhance the success of DOE's Crosscutting Research and new alloy development program and provide significant public benefits.



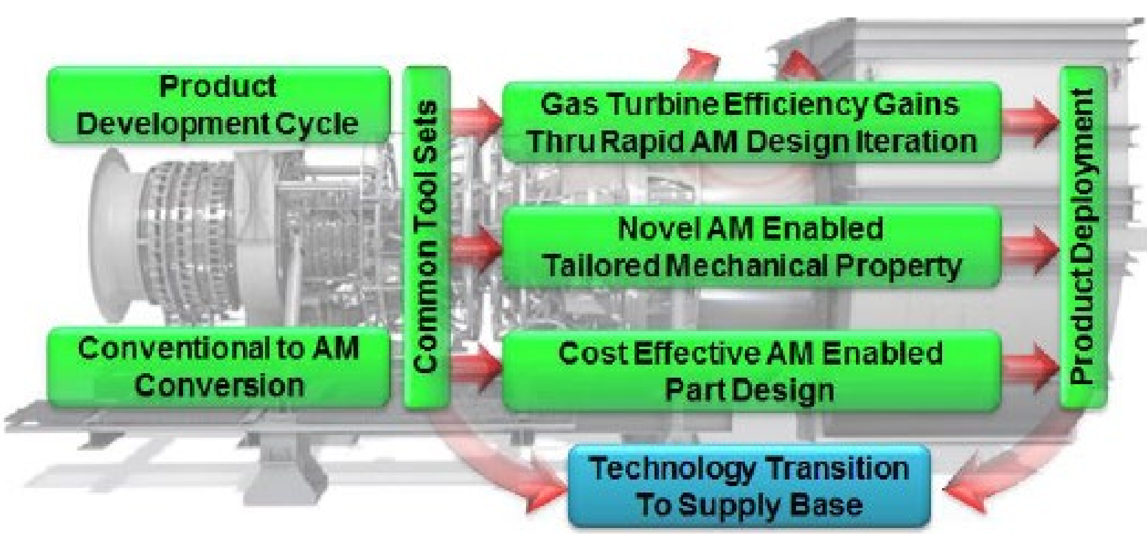
Model prediction with microstructure evolution.

Computation Tools for Additive Manufacture of Tailored Microstructure and Properties

Performer	**United Technologies Research Center**
Award Number	FE0031642
Project Duration	9/1/2018 – 8/31/2020
Total Project Value	$ 950,244
Technology Area	Coal Utilization Science

United Technologies Research Center will demonstrate the application of computational methods and tools on microstructure evolution and mechanical properties prediction for additively manufactured (AM) nickel-based superalloy parts. Models will be developed in three areas: AM process parameters–microstructure correlation models; correlation between initial microstructure and final microstructure after heat treatment; and final microstructure-to-mechanical-properties relationship. The ability to tailor spatially varying mechanical properties in part by appropriately controlling the microstructure evolution during the AM process will be demonstrated using these models. An integrated computational materials engineering framework that connects process, structure, properties, and performance will be developed and demonstrated. This project extends computational phase-field models for microstructure evolution—as a function of material processing parameters and crystal plasticity models—fully coupling microstructure, mechanical properties, and service life required for turbine engines.

The tools developed in this project will enable refurbishment of legacy F-Class industrial gas turbines with polycrystalline alloy components built additively by laser powder-bed fusion. These toolsets can be extended to future directionally solidified and single-crystal superalloys produced using AM technology. The time saved by applying validated predictive tools will allow exploration of novel concepts such as tailored property placement based on varying operational requirements within a single part, further unlocking the potential of AM hardware.



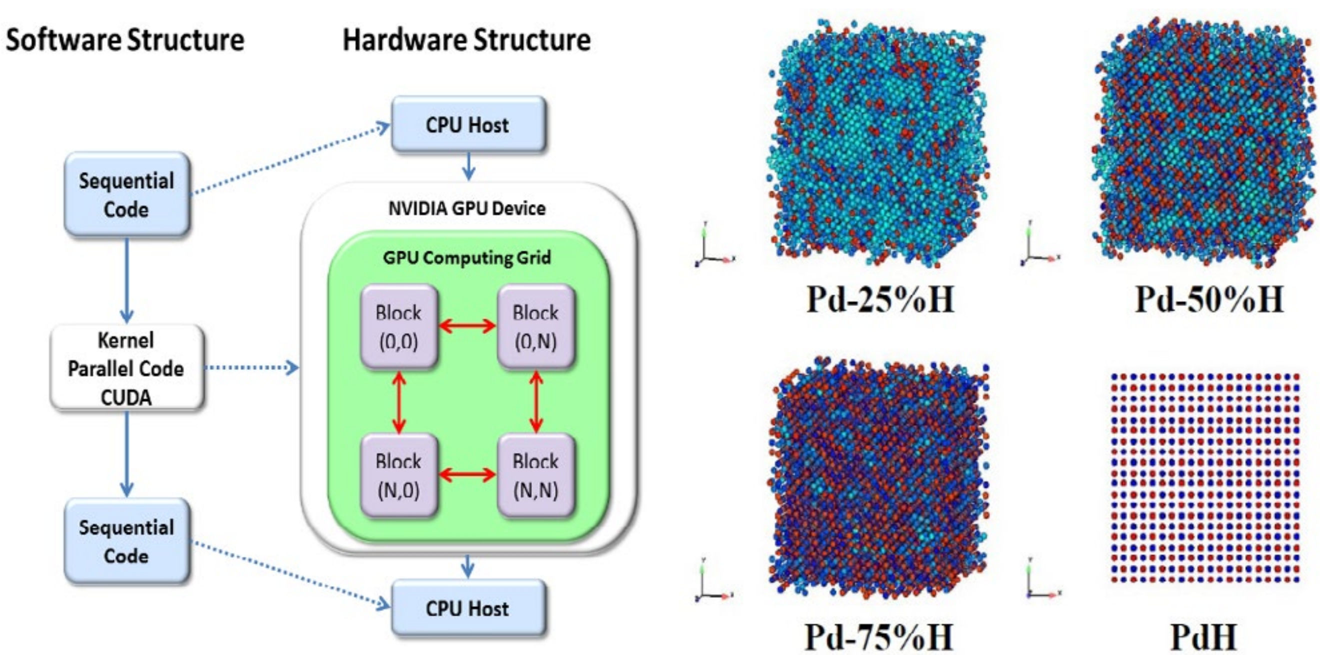
Additive manufacturing impact on industrial gas turbines.

Large-Scale, Graphics Processing Unit (GPU)-Enhanced Density Functional Tight Binding (DFTB) Approaches for Probing Multi-Component Alloys

Performer	**University of California, Riverside**
Award Number	FE0030582
Project Duration	8/1/2017 – 7/31/2020
Total Project Value	$ 250,000
Technology Area	University Training and Research

The objectives of this project are to develop, analyze, and introduce (1) accurate intermolecular potentials and (2) graphics processing unit enhancements to the density functional tight binding approach for high-throughput ab initio molecular dynamics calculations of multi-component alloys at elevated temperatures. Specifically, this transformative approach utilizes two complementary pathways that will employ a high degree of coordination and communication between them to realize a final rigorously sound and validated computational capability upon completion.

The capabilities developed in this project will provide accurate, efficient, and reduced-cost assessment of alloy structural performance at elevated temperature and pressure operational conditions in advanced fossil energy power plants.



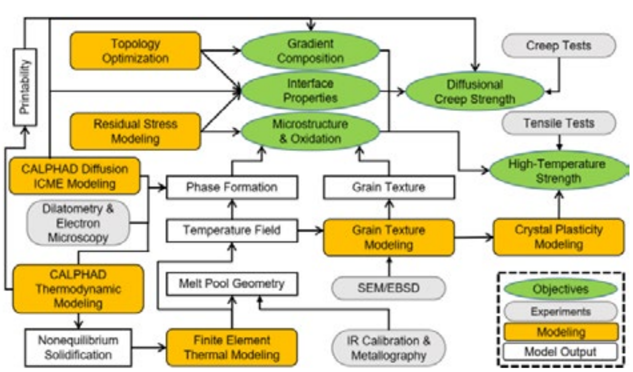
Large-scale simulations of alloy systems.

Integrated Computational Materials and Mechanical Modeling for Additive Manufacturing of Alloys with Graded Structure used in Fossil Fuel Power Plants

Performer	**University of Pittsburgh**
Award Number	FE0031637
Project Duration	11/1/2018 – 10/31/2020
Total Project Value	$ 937,500
Collaborator	United Technologies Research Center
Technology Area	Coal Utilization Science

University of Pittsburgh (Pitt) researchers will develop an integrated computational materials engineering modeling framework through a combination of materials and mechanical models for relevant advanced ultra-supercritical components and materials processed by wire-arc additive manufacturing (WAAM). Physics-based process-structure-property models will be developed to predict thermal history, melt pool geometry, phase stability, grain morphology/texture, high-temperature oxidation, tensile and creep strength, and residual stress. In addition to bulk properties for single materials, interfacial properties between two dissimilar alloys joined together will be modeled and employed to design the compositional profile in the interfacial zone using phase transformation modeling and topology optimization techniques. All the models developed will be validated by characterization experiments on both coupon and prototype samples, and their uncertainty will be quantified via sensitivity analysis. Pitt will be responsible for model development and simulation. United Technologies Research Center (UTRC) will perform sample preparation using WAAM, mechanical and tensile strength testing, high-temperature oxidation and creep tests to support calibration of the structure-property modeling. Both Pitt and UTRC will work on model calibration and verification.

Development of a simulation tool that can predict the structure-property relationships of extreme environment materials for fossil energy infrastructure manufacturing will lead to a framework and manufacturing methods that can be used in other energy unit manufacturing, such as concentrated solar power plants and ultra-supercritical and supercritical boiler systems. The developed model will support the joining of dissimilar alloys that are vitally important in the welding and joining industry; the manufacture of functionally graded alloys that are not limited to the fossil fuel energy infrastructure; and further development of an additive manufacturing technique for repairing critical fossil fuel energy generating components. Also, this project is expected to lead to the design and manufacture of superior alloy components with excellent creep-rupture strength and oxidation resistance at elevated temperatures as required for the efficient operation of fossil fuel power plants.



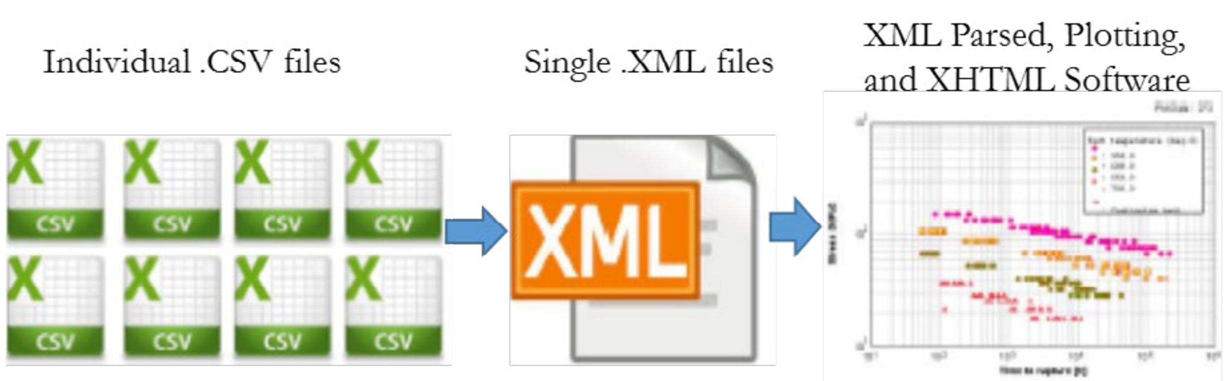
Integrated Computational Materials Engineering model framework for additive manufacturing of alloys with graded structure.

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	9/1/2016 – 8/31/2019
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 in 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.

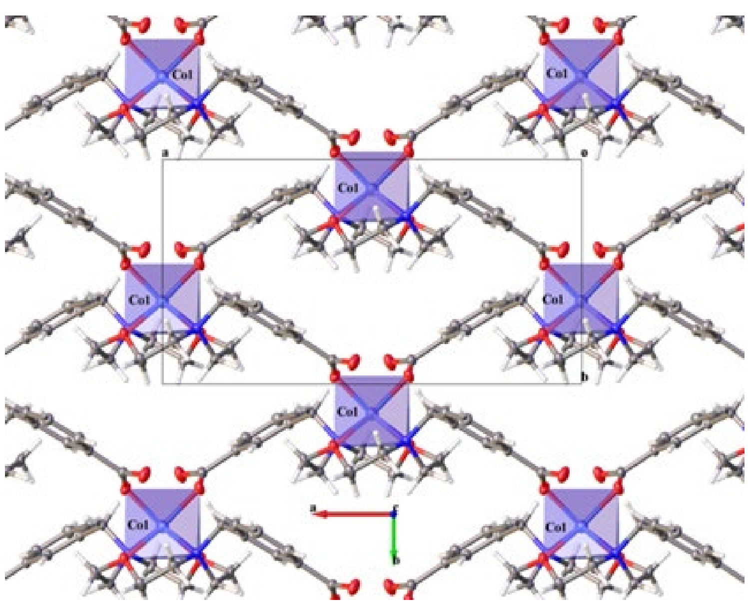
FUNCTIONAL MATERIALS FOR PROCESS PERFORMANCE

Engineering Accessible Adsorption Sites in Metal Organic Frameworks for CO_2 Capture

Performer	**Clark Atlanta University**
Award Number	FE0022952
Project Duration	10/1/2014 – 3/31/2019
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	10/1/2015 – 9/30/2021
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 (FE) goals and objectives. Research efforts will directly support FE's Coal and Oil & Natural Gas programs in a variety of program areas including advanced energy systems, CO_2 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.

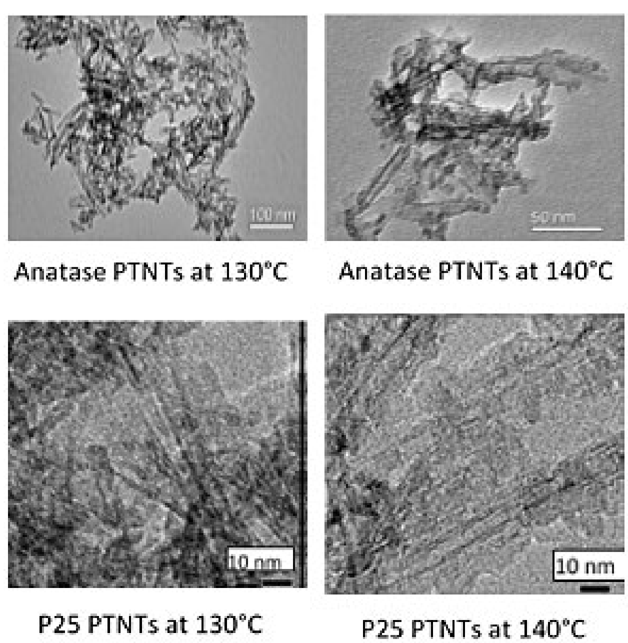
Project focuses on advancing basic and applied energy research.

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

Performer	**Prairie View A&M University**
Award Number	FE0023040
Project Duration	10/1/2014 – 3/31/2019
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 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.

ABBREVIATIONS

°C .... degrees Celsius
°F .... degrees Fahrenheit
ACT .... accelerated creep testing
AM .... additive manufacturing
ASME .... American Society of Mechanical Engineers
AUSC .... advanced ultrasupercritical
BN .... boron nitride
CALPHAD .... calculation of phase diagrams
CAU .... Clark Atlanta University
CFD .... computational fluid dynamics
CNT .... carbon nanotube
CO_2 .... carbon dioxide
CSEF .... creep strength enhanced ferritic
DARPA-AIM .... Defense Advanced Research Projects Agency - Accelerated Insertion of Materials
DFT .... density functional theory
DFTB .... density functional tight binding
DNV .... Det Norske Veritas
DOE .... Department of Energy
DofE .... design of experiments
DTMM .... digital twin material model
EEM .... extreme environment material
FCC .... face-centered cubic
FE .... Office of Fossil Energy
FSW/P .... friction stir welding and processing
FWP .... Field Work Proposal
GB .... grain boundary
GPU .... graphics processing unit
H282 .... Haynes 282
HBCU .... Historically Black Colleges and Universities
HPM .... High Performance Materials
HX .... Hastelloy X
ICME .... integrated computational materials engineering
ICWE .... integrated computational welding engineering
INL .... Idaho National Laboratory
LP .... laser processing
MHD .... magnetohydrodynamic
MOF .... metal organic framework
MOOSE .... Multiphysics object-oriented simulation environment
MWe .... megawatts electric
NETL .... National Energy Technology Laboratory
ODS .... oxide dispersion strengthened
OMI .... Other Minority Institutions
ORNL .... Oak Ridge National Laboratory
PEI .... polyethylenimine
Pitt .... University of Pittsburgh
PNNL .... Pacific Northwest National Laboratory
psi .... pounds per square inch
R&D .... research and development
RDE .... rotating detonation engine
sCO_2 .... supercritical carbon dioxide
SE&A .... systems engineering and analysis
SHS .... self-propagating high-temperature synthesis
SwRI .... Southwest Research Institute
UCR .... University Coal Research
UTRC .... United Technologies Research Center
WAAM .... wire-arc additive manufacturing
γ' .... gamma prime
η .... eta

NOTES

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WEBSITES:

https://netl.doe.gov/coal/program124

https://netl.doe.gov/onsite-research/materials

https://netl.doe.gov/coal/crosscutting

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

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