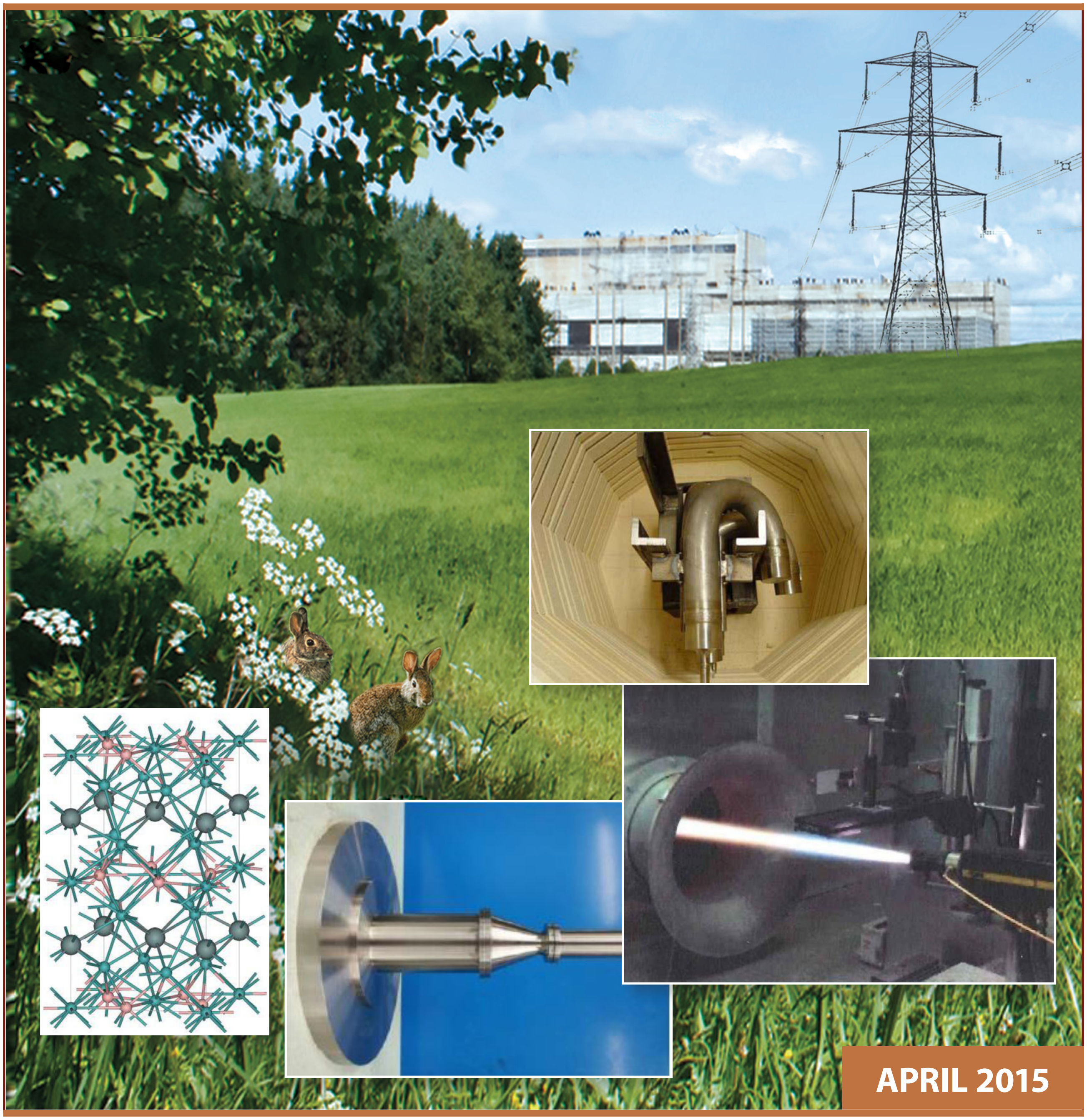
Crosscutting Technology Research High Performance Materials Project Portfolio



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the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

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Introduction

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

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

The Program comprises three technology areas: Coal Utilization Sciences, Plant Optimization Technologies, and University Training and Research. A general description of each of these technology areas is detailed below:

Coal Utilization Sciences: The Coal Utilization Sciences technology area research effort is conducted to develop modeling and simulation technologies leading to a suite of products capable of designing and simulating the operation of next-generation near-zero-emissions power systems such as gasification and oxy-combustion. These products are based on validated models and highly detailed representations of equipment and processes. Multinational laboratory efforts are being coordinated through the National Risk Assessment Partnership (NRAP) and Carbon Capture Simulation Initiative (CCSI) to focus on post-combustion capture of carbon, risk assessment, and integrated multiscale physics-based simulations.

Plant Optimization Technologies: The Plant Optimization Technologies technology area exists to develop advanced sensors and controls, materials, and water- and emissions-related technologies. Projects within this funding area enable novel control systems to optimize operations where harsh environmental conditions are present in both current and future applications in power plants and industrial facilities.

University Training and Research: The University Training and Research (UTR) program awards research-based educational grants to U.S. universities and colleges in areas that benefit the Office of Fossil Energy and the Crosscutting Technology Research Program. UTR is the umbrella program under which the University Coal Research (UCR) and Historical Black Colleges and Universities (HBCU) and Other Minority Institutions (OMI) initiatives operate. These grant programs address the scientific and technical issues key to achieving Fossil Energy's goals, and build our nation's capabilities in energy science and engineering by providing hands-on research experience to future generations of scientists and engineers.

In addition to the Crosscutting Technology Research funding programs listed above, NETL uses its participation in the U.S. Department of Energy's (DOE) Office of **Science Small Business Innovation Research (SBIR) Program** to leverage funding, enhance the research portfolio, and most importantly, facilitate a pathway to commercialization. SBIR is a highly competitive program that encourages small businesses to explore technological potential and provides the incentive to profit from commercialization. By including qualified small businesses in the nation's

R&D arena, high-tech innovation is stimulated and the United States gains entrepreneurial spirit to meet specific research and development needs. SBIR targets the entrepreneurial sector because that is where most innovation and innovators thrive. By reserving a specific percentage of Federal R&D funds for small business, SBIR protects the small business and enables competition on the same level as larger businesses. SBIR funds the critical startup and development stages and it encourages the commercialization of the technology, product, or service, which, in turn, stimulates the U.S. economy. Since its inception in 1982 as part of the Small Business Innovation Development Act, SBIR has helped thousands of small businesses to compete for Federal research and development awards. These contributions have enhanced the nation's defense, protected the environment, advanced health care, and improved our ability to manage information and manipulate data.

The Crosscutting Technology Research program comprises these key technology areas:

Sensors and Controls: The basis for this research area is to make available new classes of sensors and measurement tools that manage complexity, permit low cost, robust monitoring, and enable real-time optimization of fully integrated, highly efficient power-generation systems. Controls research centers around self-organizing information networks and distributed intelligence for process control and decision making.

High Performance Materials: Materials development under the Crosscutting Technology Research Program focuses on structural materials that will lower the cost and improve the performance of fossil-based power-generation systems. Computational tools in predictive performance, failure mechanisms, and molecular design of materials are also under development to support highly focused efforts in material development.

Simulation-based Engineering: This technology area represents a vast amount of expertise and capability to computationally represent the full range of energy science from reactive and multiphase flows up to a full-scale virtual and interactive power plant. Science-based models of the physical phenomena occurring in fossil fuel conversion processes and development of multiscale, multi-physics simulation capabilities are just some of the tools and capabilities under this technology area.

Innovative Energy Concepts: Innovative Energy Concepts is concerned with the development of novel cost-effective technologies that promote efficiency, environmental performance, availability of advanced energy systems, and the development of computational tools that shorten development timelines of advanced energy systems. This area provides for fundamental and applied research in innovative concepts with a 10-25 year horizon that offers the potential for technical breakthroughs and step-change improvements in power generation and the removal of any environmental impacts from fossil energy-based power system.

Water Management Research and Development: Water research encompasses the need to reduce the amount of freshwater used by power plants and to minimize any potential impacts of plant operations on water quality. The vision for this program area is to develop a 21st-century America that can count on abundant, sustainable fossil energy and water resources to achieve the flexibility, efficiency, reliability, and environmental quality essential for continued security and economic health. To accomplish this, crosscutting research is needed to lead a critical national effort directed at removing barriers to sustainable, efficient water and energy use, developing technology solutions, and enhancing understanding of the intimate relationship between energy and water resources.

High Performance Materials

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

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

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

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

Specific Technology Objectives:

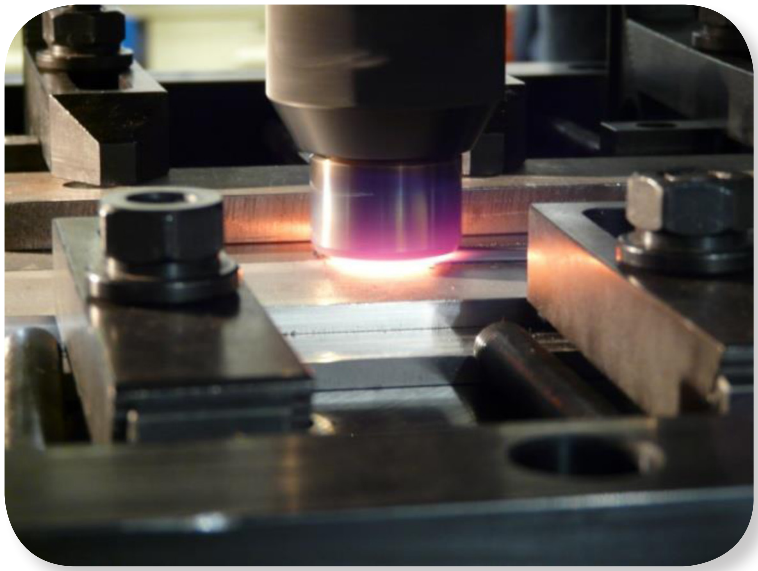
- Development of computational materials modeling to enable rapid design and simulation of new and novel alloy materials with less repetitive testing. Computational design of materials has the potential to produce major breakthroughs.
- Development of superalloys and ferritic materials for use in AUSC 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.
- Development of functional materials for energy storage and high-performance materials with mechanical properties that can perform reliably at temperatures well over 1,000 °C
- Development of advanced metallic and ceramic coatings, including nanomaterials, to provide thermal barrier protection for turbine blades, combustor components and tubing.
- Validated computational models capable of simulating and predicting performance of materials in various types of transformational power plants, including pressurized oxy-combustion, pressurized gasification, and carbon dioxide (CO_2) cycle plants.

This project portfolio report showcases 61 high-performance materials projects within the Crosscutting Research Program of the Strategic Center for Coal. Each of the pages reporting on projects clearly describes the technology, the program goals, and overall benefits.

Projects by Research Area

Advanced Manufacturing

The objective of the Coatings/Protection Materials research area is to develop the design, application, and performance criteria for coatings intended to protect materials from the high-temperature corrosive environments encountered in advanced fossil energy plants.



Friction stir welding of 1/4" thick dispersion strengthened Sandvik APMT plate.

Improved Atomization Processing for Fossil Energy Applications

Performer: Ames National Laboratory

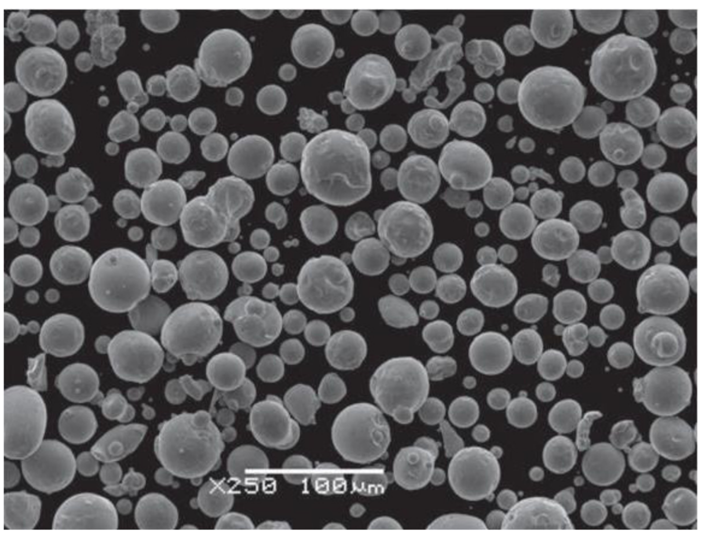
Award Number: FWP-AL-14-510-070

Project Duration: 10/1/2013 – 9/30/2014

Total Project Value: $75,000

Technology Area: Plant Optimization Technologies

NETL partnered with Ames National Laboratory to enhance the control of metal powder production by gas atomization methods to benefit the implementation of several emerging Fossil Energy technologies that utilize metal powders of specific size ranges and types not efficiently produced by industrial powder makers. Improvements in fundamental understanding and design of high efficiency gas atomization nozzles were directed toward maximizing powder yields in special size classes, including ultrafine (diameter less than 10 µm) and mid-range (diameter between 10 µm and 44 µm) powders. Efficient production of such powders can eliminate a major technological barrier to the use of new concepts for fabrication, for example, hydrogen membranes, heat exchanger tubing, and oxidation/ sulfidation resistant coatings. To provide a direct route for rapid transfer of the atomization technology improvements, powder production tests were performed in laboratory atomization systems that were relevant to industrial processes in terms of steady-state operation and controls systems. The laboratory atomization experiments also involved detailed analysis of atomization process response to alloy and parameter modifications to verify the effect of process innovations.



Atomized powder.

Additive Manufacturing for Cost Efficient Production of Compact Ceramic Heat Exchangers and Recuperators

Performer: Ceralink Inc.

Award Number: FE0024066

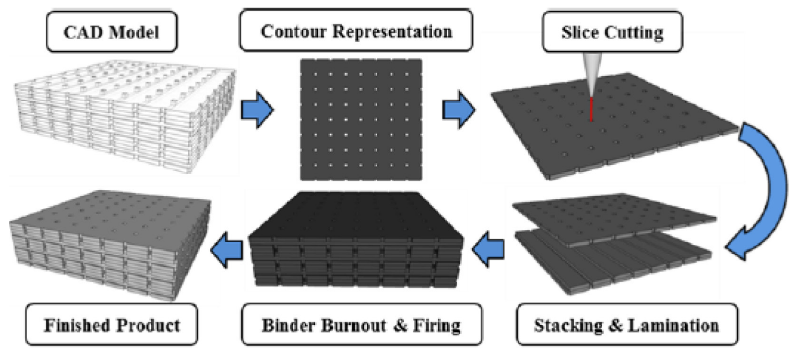
Project Duration: 11/1/2014 – 10/31/2015

Total Project Value: $639,345

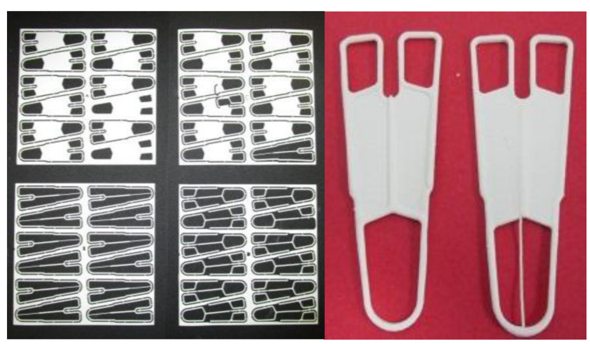
Technology Area: Plant Optimization Technologies

NETL is partnering with Ceralink Inc. to design and build a prototype high-temperature and compact ceramic heat exchanger, based on the laminated object manufacturing (LOM) technique, as a key component for high efficiency advanced power generation systems.

The objective of this project is to design and build a prototype compact high-temperature ceramic heat exchanger as a key component for high efficiency advanced power generation systems. Specifically, several mature and emerging technologies will be combined to develop a novel high thermal conductivity aluminum nitride based heat exchanger. The target prototype will reduce the weight to volume ratio by 60% compared to metal heat exchangers and will allow operation well above 1500 °F (816 °C). Selecting a ceramic material over standard metal will allow a much more compact size, as well as higher operating temperatures. The project will lead to an estimated 25% increase in system level recuperator thermal efficiency, energy savings in aerospace, distributed combined heat and power generation and will provide reductions in CO_2, NO_X, and SO_X emissions.



LOM builds 3D parts from 2D ceramic tapes.



Ceramic layers for Naval Research Lab compact micro recuperator.

Compact, Ceramic Microchannel Heat Exchangers

Performer: Ceramatec Inc.

Award Number: FE0024077

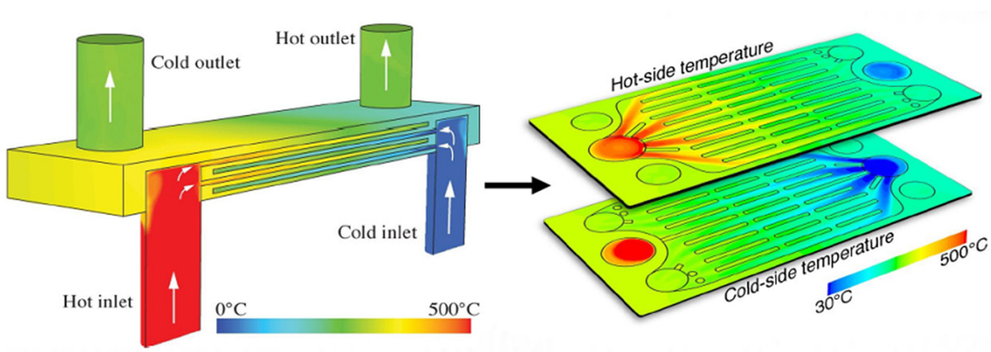
Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $499,922

Technology Area: Plant Optimization Technologies

NETL is partnering with Ceramatec to obtain performance data for prototype compact ceramic microchannel heat exchangers capable of improving power plant efficiency. Ceramatec will collaborate with Colorado School of Mines (CSM) to meet the project objectives. Ceramatec will be responsible for fabricating and testing heat exchanger plates and stacks using its unique microchannel manufacturing capabilities, while CSM will derive heat exchanger plate specifications from system requirements using numerical power systems modeling approaches such as ASPEN. Subsequently, CSM will work with Ceramatec to design the microchannel architecture for a heat exchanger plate that will be the basic repeat unit of heat exchanger stacks. CSM will perform 3-D computational fluid dynamics using numerical modeling tools such as FLUENT. Test results will be used as feedback to iterative design modifications. These activities will define a heat exchanger plate design for stack testing. Ceramatec will fabricate heat exchanger plates and assemble them into stacks capable of 1-5 kWth duty and integrate the stacks with appropriate manifolds and thermal systems for subsequent testing at elevated temperature.

Development of compact ceramic microchannel heat exchangers will enable higher operating temperatures in power plants that will lead to higher efficiency and reduced emissions.



Heat exchanger plate design and analysis.

Additive Manufacturing of Fuel Injectors

Performer: Edison Welding Institute, Inc.

Award Number: FE0023974

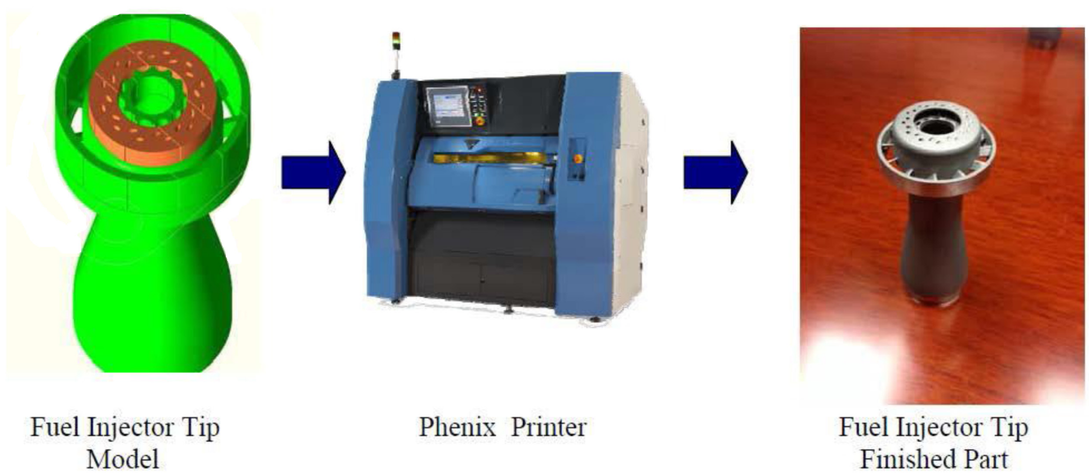
Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $622,384

Technology Area: Plant Optimization Technologies

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

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



50,000 foot view of AM Courtesy of EWI.

Benefits of Hot Isostatic Pressure/Powdered Metal (HIP/PM) and Additive Manufacturing (AM) to Fabricate Advanced Energy System Components

Performer: Energy Industries of Ohio Inc.

Award Number: FE0024014

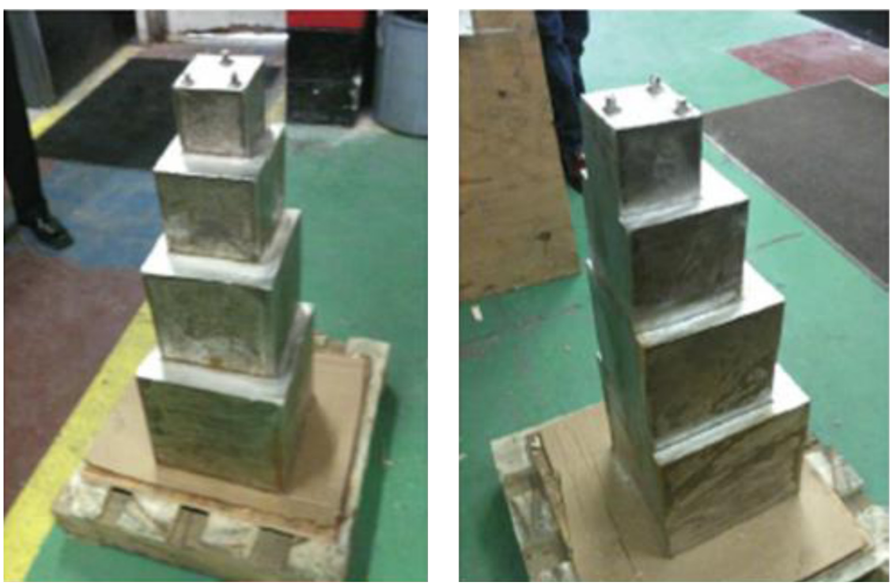
Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $625,000

Technology Area: Plant Optimization Technologies

NETL is partnering with Energy Industries of Ohio Inc to demonstrate that tailoring Hot Isostatic Pressure of Powdered Metal (HIP/PM), coupled with advances in additive manufacturing (AM), has specific, measurable benefits for fabricating advanced energy system components. The objectives for the project include production of (1) fully dense test coupons to determine the requisite material characterization and sintering protocols and (2) two HIP cans in Haynes 282 with different wall thicknesses, and (3) analysis of valve parts for chemical and material properties.

Benefits of this project include validation of AM (combining 3-D printing and HIP) as a viable method of producing Haynes 282 components as well as providing key information about cost, manufacturing challenges/opportunities and lead-times when compared to other methods including HIP/PM and casting.



A Haynes 282 step component that has been duplicated using HIP/PM.

High Temperature Ceramic Heat Exchanger for Solid Oxide Fuel Cell

Performer: Mohawk Innovative Technology, Inc.

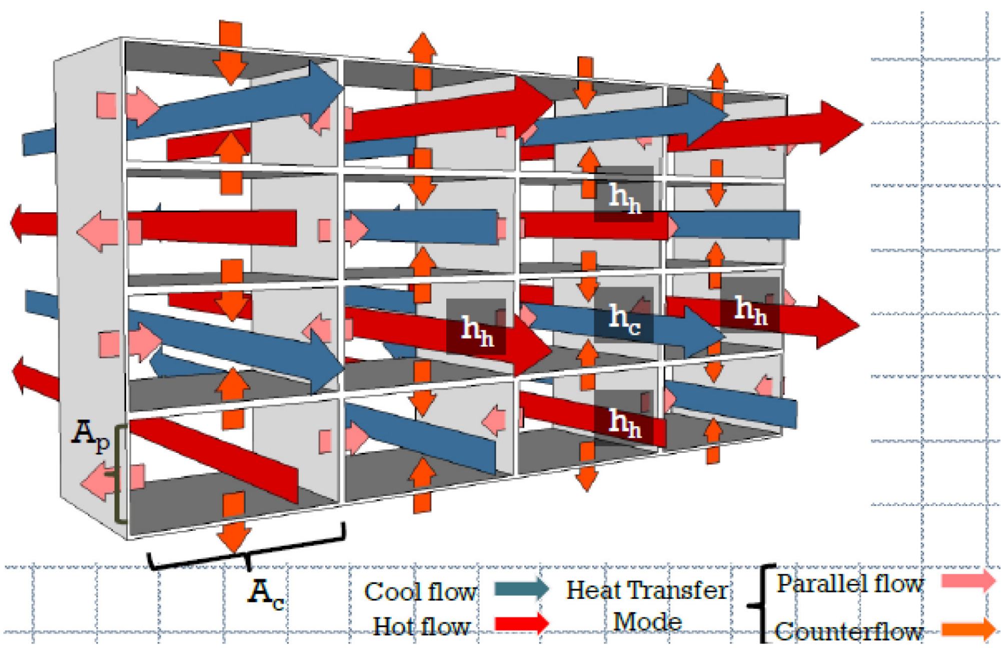
Award Number: FE0024090

Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $643,682

Technology Area: Coal Utilization Sciences

NETL is partnering with Mohawk Innovative Technology, Inc. to develop a ceramic heat exchanger with high effectiveness and low pressure drop to work as a preheater for solid oxide fuel cell (SOFC) application. The objectives for the project include R&D work to select a design, material, and fabrication method for the heat exchanger followed by component tests under relevant SOFC conditions. This project will lead to the development of an advanced manufacturing technique for ceramic materials.



Recuperator Geometry.

Low Cost Fabrication of ODS Materials

Performer: Pacific Northwest National Laboratory (PNNL)

Award Number: FWP-60098

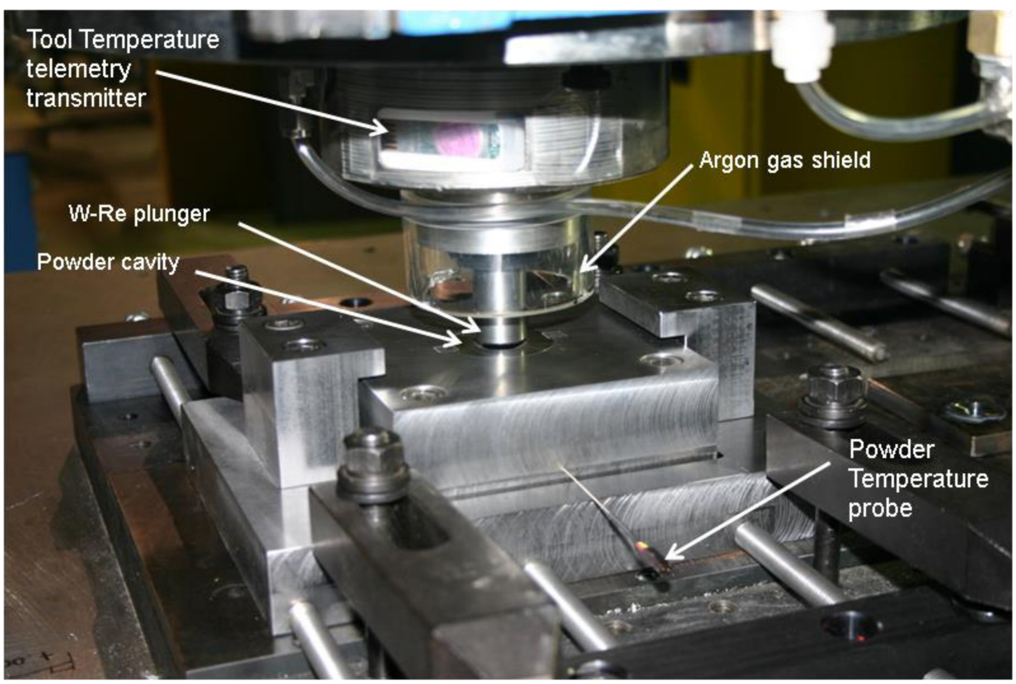
Project Duration: 10/1/2010 – 9/30/2015

Total Project Value: $570,000

Technology Area: Plant Optimization Technologies

NETL is partnering with PNNL to develop a process to fabricate oxide dispersion-strengthened (ODS) materials at lower cost than current manufacturing methods used on 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 objective of this project is to develop a low-cost method for producing high-strength, creep resistant ODS ferritic steel mill product for high-temperature applications. This project will contribute to more efficient use of fossil fuels in AUSC power plants, which will concurrently lead to reduced discharge of carbon dioxide and other emissions.



Friction Extrusion Die at Pacific Northwest National Laboratory.

Solid State Joining of Creep Enhanced Ferritic Steels

Performer: Pacific Northwest National Laboratory (PNNL)

Award Number: FWP-66059

Project Duration: 10/1/2014 – 9/30/2015

Total Project Value: $300,000

Technology Area: Plant Optimization Technologies

NETL is partnering with PNNL to develop an alternative solid state joining technology, friction stir welding (FSW), which can enable higher performance from creep strength enhanced ferritic (CSEF) steels, anticipated to be used in advanced ultrasupercritical (A-USC) coal-fired power plants. A primary problem in the high-temperature application of welded CSEF steels is that the welds of these steels fail (Type IV cracking) at a creep life far below that of the base metal. This has led to a reduced performance envelop and either a calculation of reduced strength and lifetime for assemblies made from these alloys, or the use of expensive post-weld heat treatment (PWHT) 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 has the ability to produce 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 advanced ultrasupercritical coal-fired power plants will improve efficiency and operational flexibility, and result in lower operating costs.

Flat plate FS welds in HSLA65 plate, stay flat!

A Computational Experimental Study of the Plasma Processing of Carbides at High Temperatures

Performer: University of Texas at El Paso

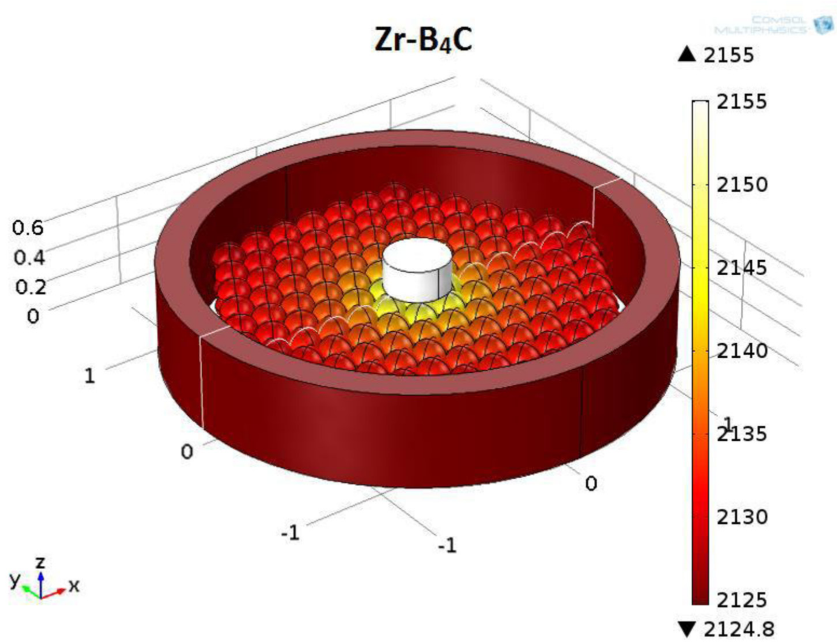
Award Number: FE0008400

Project Duration: 7/1/2012 – 6/30/2015

Total Project Value: $200,000

Technology Area: University Training and Research

NETL is partnering with the University of Texas at El Paso to investigate computationally the plasma processing with strategic experimentation of SiC, ZrC-TiC-Y2O$_3$ and Ti_2AlC-TiC-Y_2O_3 packed beds, which ultimately will form SiO_2, ZrO_2-TiO_2- Y_2O_3, and Al_2O_3-Al_2TiO_5-Y_2O_3 scales for high temperature materials. The focus of the study is in understanding sufficiently plasma processing of nonmetallic packed beds for developing materials for extreme temperatures, such as materials with protective oxidizing scales operational at temperatures greater than 1773 kelvin (K). The plasma processing operating at 1973 to 2500 K for the carbides and their oxidation at 1973 K will involve the following research objectives: (1) investigate the effects of the plasma flow dynamics within the pores to form oxycarbide and amorphous phases, which ultimately would impede oxygen ingress through a packed bed or a protective scale; (2) determine the effect of the potential gradient established by the electromagnetic field on sealing pores as a result of the temperature spikes on pore surfaces; and (3) investigate the surface kinetics within the pore wall of the packed bed as a result of the plasma coupling mass and heat transport.



Three-dimensional view of carbide spheres used to simulate heat transfer with COMSOL Multiphysics.®

Design Optimization of Liquid Fueled High Velocity Oxy-Fuel Thermal Spraying Technique for Durable Coatings for Fossil Power Systems

Performer: University of Texas at El Paso

Award Number: FE0008548

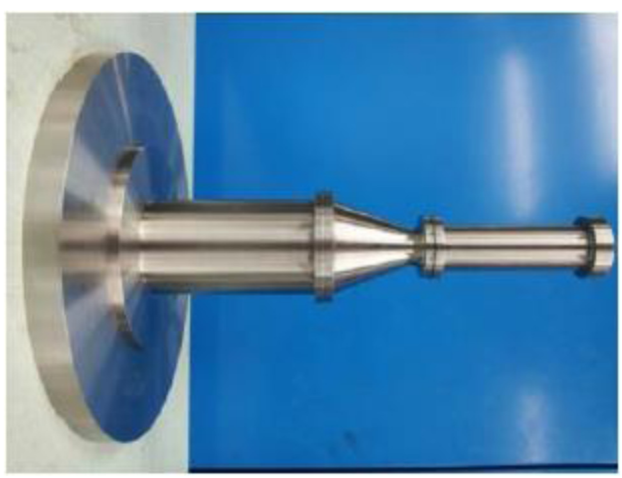
Project Duration: 7/1/2013 – 6/30/2015

Total Project Value: $200,000

Technology Area: University Training and Research

NETL is partnering with the University of Texas at El Paso to understand the relationship between process parameters of the liquid-fueled high velocity oxy-fuel (LHVOF) thermal spray technique and coating durability in order to optimize the technique's effectiveness. The first objective of the project is to determine the particle dynamics of the LHVOF process for a range of operating and process parameters. The microstructural and physical characteristics of LHVOF-produced coatings are critically dependent on the physical and chemical states and dynamics of the coating particles. The second objective is to determine the effects of the operating and process parameters on coating characteristics. The effects of process and operating conditions on the overall growth and micro/nano-structural evolution of three types of coatings will be systematically studied. Researchers will investigate the relative importance of various thermo-mechanical and thermo-chemical failure modes of the coatings by exposing them to test environments containing relevant gases (oxygen, steam, and oxides of sulfur) at high temperature. A high-pressure combustor rig will be used to determine how thermal stress cycling, oxidation degradation, and their complex interactions can cause coating failures.

A comprehensive understanding of the physical and thermo-chemical processes of the LHVOF system and how they interact with coating materials will enable new technology innovation and finer quantitative control of coating performance to meet stringent requirements for use in advanced ultra-supercritical boiler, steam turbine, and gas turbine operational environments.



UTEP developed HVOF gun for high temperature coatings.

Mechanically Activated Combustion Synthesis of $MoSi_2$-Based Composites

Performer: University of Texas at El Paso

Award Number: FE0008470

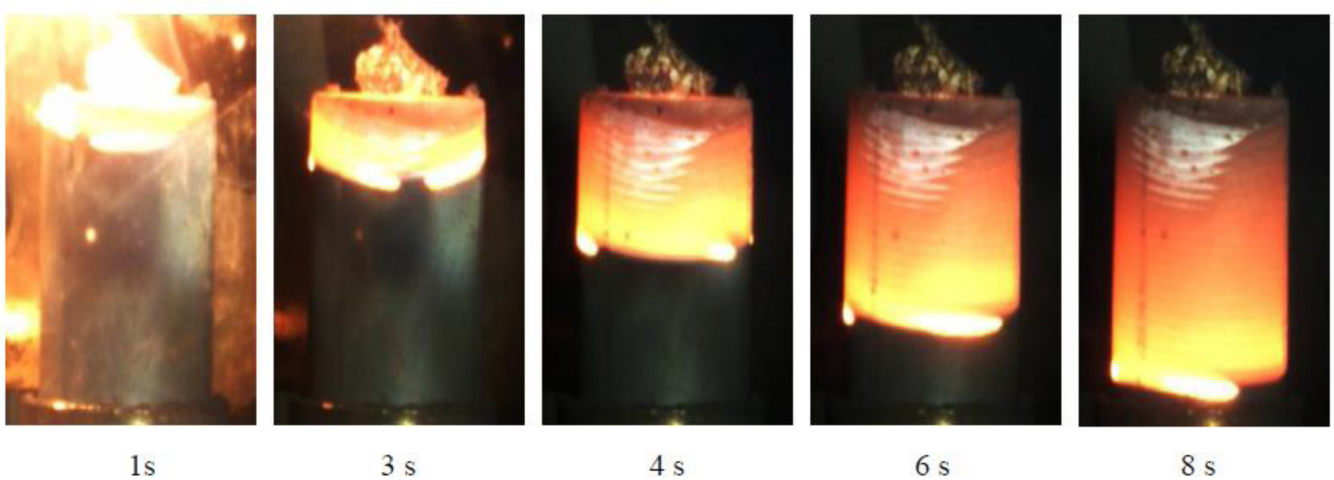
Project Duration: 7/1/2012 – 6/30/2015

Total Project Value: $236,000

Technology Area: University Training and Research

NETL is partnering with the University of Texas at El Paso to develop a novel and competitive processing route for manufacturing $MoSi_2$-based composites, which are promising materials for structural applications under operating conditions that take place in advanced boilers, steam turbines, and gas turbines. Specifically the team is investigating mechanically activated self-propagating high-temperature synthesis (MASHS) followed by compaction. The objectives of the proposed research include: (1) determination of optimal MASHS conditions for production of $MoSi_2$ reinforced with secondary phases; (2) development of an SHS compaction technique for densification and shaping of $MoSi_2$-based composites obtained by MASHS; (3) and determination of mechanical and oxidation properties of $MoSi_2$-based composites produced by MASHS-compaction.

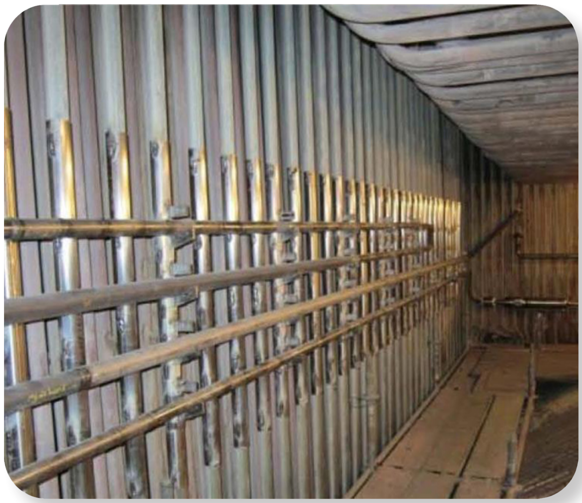
This project will produce a variety of high-quality $MoSi_2$-based composites obtained as dense, low-porous materials of various shapes that could be used for structural applications in advanced fossil fuel power plants. The project will also promote research and education of Hispanic students in the area of high-performance materials for fossil energy applications.



Spin combustion of Mo-Si-B mixture.

Advanced Structural Materials

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



High temperature oxidation/corrosion test loop for advanced structural alloys.

Advanced Ultrasupercritical (AUSC) Tube Membrane Panel Development

Performer: Alstom Power, Inc

Award Number: FE0024076

Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $666,667

Technology Area: Plant Optimization Technologies

NETL is partnering with Alstom Power Inc. to develop the design, and manufacturing processes that are required for welded tube membrane panels in power boilers for Advanced Ultra Supercritical (AUSC) steam cycles. This effort is required prior to building an AUSC Component Test facility to demonstrate high temperature, high pressure (up to 760 °C [1400 °F] and 35MPa (5000psi) steam conditions. Steam cycles operating at AUSC steam conditions can achieve a 10 percent increase in efficiency above current commercially available state-of-the-art USC boiler steam cycles at 29MPa/ up to 620 °C (4200 psi/1150 °F).

Development of high-performance materials technology will enable higher efficiency fossil energy power plants to realize more than a 10% increase in efficiency above today's state-of-the-art boiler steam cycles. The project is intended to develop and prove the manufacturability of welded tube membrane panels made from high-performance materials suitable for the AUSC steam cycles (greater than 1300 °F / 4000psi) of a fossil-fired boiler.

Straight flat panels in shop.

Boiler wall layout in shop.

Component Test Facility (COMTEST) Phase 1 Engineering for 760 °C (1400 °F) Advanced Ultrasupercritical (A-USC) Steam Generator Development

Performer: Babcock & Wilcox Power Generation Group, Inc.

Award Number: FE0024067

Project Duration: 10/1/2014 – 12/31/2015

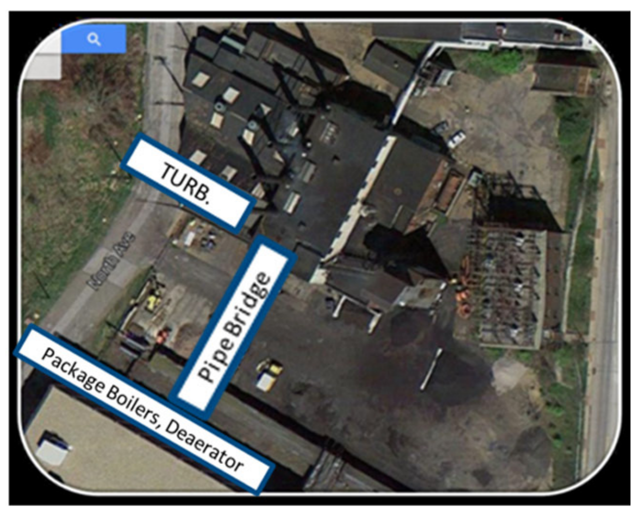
Total Project Value: $658,422

Technology Area: Plant Optimization Technologies

NETL is partnering Babcock & Wilcox Power Generation Group, Inc. to perform the pre-front end engineering design (Pre-FEED) of a gas fired A-USC steam superheater capable of operating at 760 degrees Celsius (˚C) steam temperature. The superheater would be part of a future A-USC component test program. The pre-front end engineering design package will include data definition, systems evaluation and materials/components selection that would be needed to complete final engineering design of the A-USC steam superheater in an A-USC component test facility. Plans for the steam superheater manufacturing, construction, commissioning, operation and testing will also be developed in this project.

This work is expected to reduce the economic risk of the first A-USC demonstration plant.

T-92 test wall panel.



ComTest Youngstown Thermal.

Predicting the Oxidation/Corrosion Performance of Structural Alloys in Supercritical CO_2

Performer: Electric Power Research Institute Inc.

Award Number: FE0024120

Project Duration: 10/1/2014 – 9/30/2016

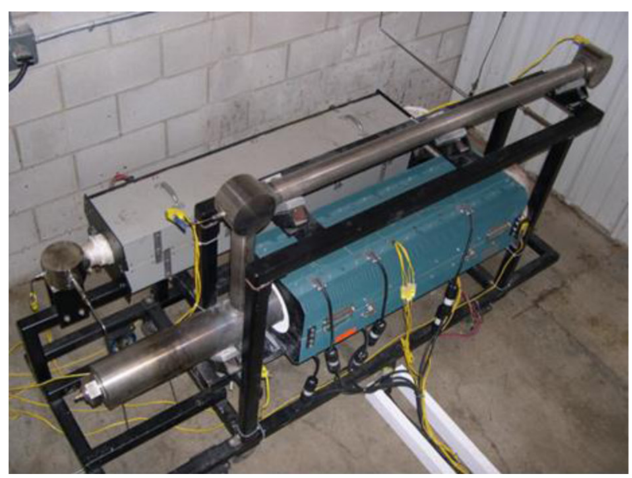
Total Project Value: $571,185

Technology Area: Plant Optimization Technologies

NETL is partnering with the Electric Power Research Institute to develop an oxidation/corrosion model to predict the performance of structural alloys in terms of oxide growth rate and tendency for scale exfoliation in supercritical CO_2 in severe operating environments at high temperatures. This goal will be accomplished by (1) short-term isothermal lab-scale oxidation/corrosion tests in high-pressure (200 atmosphere [atm] or higher) and high-temperature (650-750 degrees Celsius) supercritical $CO_{2,}$ (2) characterization of the oxide scales on the exposed samples and determination of the oxide scale growth and exfoliation kinetics, and (3) modeling of the process of oxide growth and exfoliation with and without heat-flux, and application of the model to actual tube geometries. A longer-term exposure on a relevant geometry will also be conducted as a confirmatory test for the developed model. Using the model results, recommendations will be made for structural materials selection for alloys in high-temperature supercritical CO_2 environments.

It is anticipated that the research will lead to improved confidence in materials selection for high temperature CO_2 heat-exchangers. It may also ensure that materials can achieve the desired conditions for high efficiency. The work may lead to streamlined testing and/or improved criteria for materials selection based on oxidation/corrosion and could provide key data needed by heat-exchanger manufacturers.

Procured steel materials identified for testing.



Task 3 test rig.

Development of Advanced Materials for Ultrasupercritical Boiler Systems

Performer: Energy Industries of Ohio Inc.

Award Number: FG26-NT41175

Project Duration: 10/1/2001 – 9/30/2015

Total Project Value: $33,179,639

Technology Area: Plant Optimization Technologies

NETL is partnering with Energy Industries of Ohio, Inc. to identify and develop technologies needed for operating steam cycles in coal-fired power plants at USC temperatures. The project encompasses a wide ranging effort to define and evaluate materials operating under these conditions.

The research primarily aims at identifying materials that limit operating temperatures and thermal efficiency of coal-fired plants; defining and implementing ways of producing improved alloys, fabrication processes, and coating methods that allow boilers to operate at USC conditions; participating in the certification process of the American Society of Mechanical Engineers (ASME) and generating data to lay the groundwork for ASME code approval of these alloys; defining issues affecting the design and operation of USC plants; and developing cost targets.

The anticipated benefit will be the ability to identify advanced materials to maintain a cost-competitive, environmentally acceptable coal-based electricity generation option and aid in the construction of high-efficiency coal fired power plants.

Corrosion due to steamside oxidation.

Fireside corrosion during in-plant testing with high-sulfur coal.

Steam Turbine Materials for Advanced Ultrasupercritical (AUSC) Coal Power Plants

Performer: Energy Industries of Ohio, Inc.

Collaborator(s): ALSTOM Power Inc., Electric Power Research Institute, GE Energy Inc.

Award Number: FE0000234

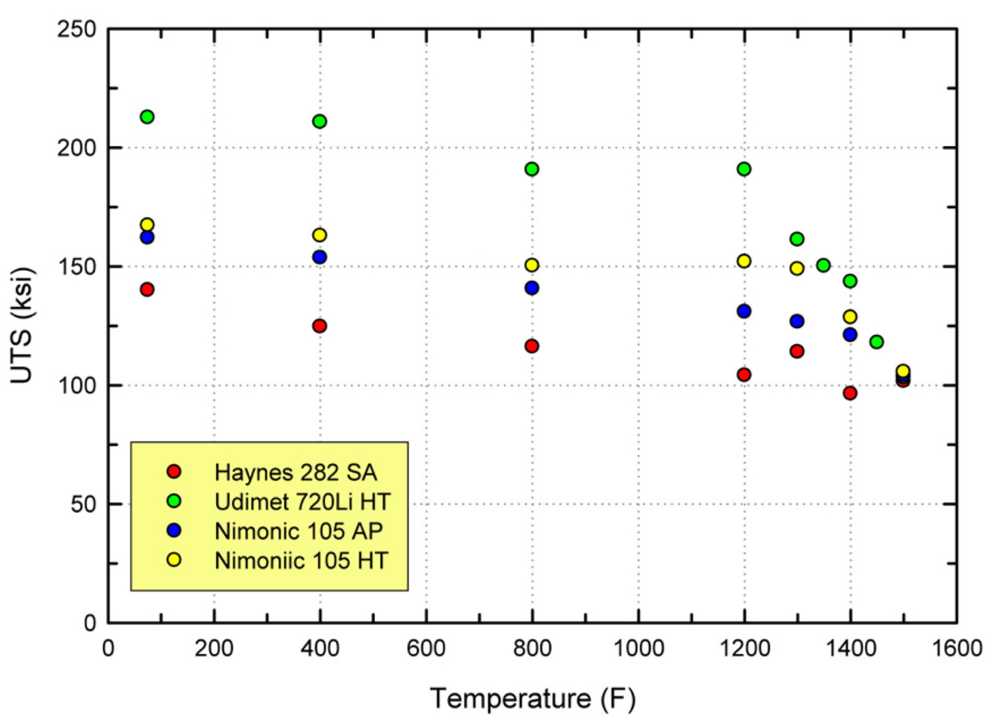
Project Duration: 10/1/2009 – 9/30/2015

Total Project Value: $11,041,018

Technology Area: Plant Optimization Technologies

NETL is partnering with Energy Industries of Ohio, Inc. to develop materials technology for AUSC steam turbines that matches the technology being developed for use at USC boiler conditions. This is a priority step before full-scale demonstration and eventual commercialization of AUSC power plants. This project follows a three-year preliminary evaluation that identified a wide spectrum of alloys and coatings. Preliminary evaluations of a subset of promising materials were completed, including research on the mechanical properties, oxidation resistance, weldability, and suitability of alloys and coatings. This project will support in-depth, longer term testing to provide materials characterization data necessary for the design of a steam turbine operable in advanced USC conditions.

The objective is to contribute to the development of materials technology for use in AUSC pulverized coal power plants capable of operating at steam temperatures up to 760 °C (1400 °F) and pressures to 35 megapascals (MPa) [5000 pounds per square inch (psi)]. This project is expected to contribute to the development of materials technology for use in power plant steam turbines capable of operating in coal-fired plants at high temperature and pressure AUSC and USC operating conditions.



UTS as a function of temperature for Haynes 282 SA, Udimet 720Li HT, Nimonic 105 AP, and Nimonic 105 HT.

Computational Aspects in Alloy Design & Life Prediction

Performer: NETL-ORD

Award Number: IPT_FY15 (task 3.4)

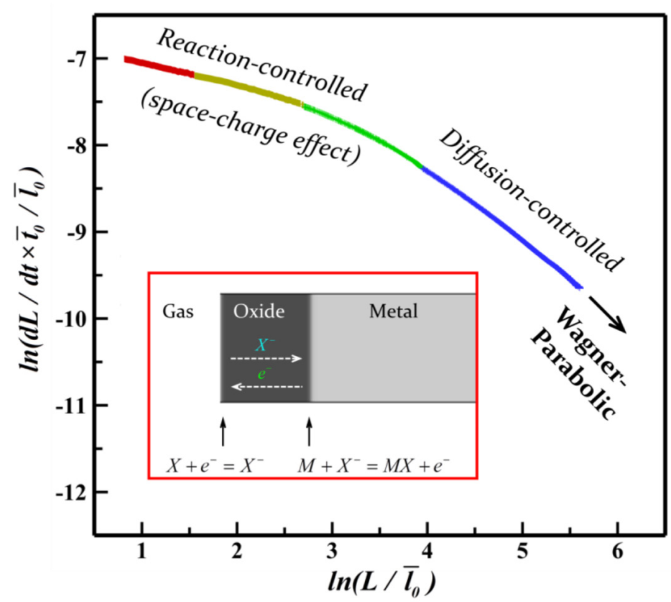
Project Duration: 10/1/2014 – 9/30/2015

Total Project Value: $500,000

Technology Area: Plant Optimization Technologies

Computational high-throughput computing methodologies will be used to identify promising alloy compositions and/or matrix compositions (e.g., those based on high-entropy concepts) for improving the performance of ferritic/martensitic steels, austenitic stainless steels, nickel base superalloys, and new and unique metallic alloy systems that extend temperature (>15 °C over existing equivalent commercial alloys) and/or strength capabilities (>10% improvement in yield strength over existing equivalent commercial alloys) for advanced FE systems.

This project will continue development of existing computational models (e.g., oxidation) by adding realistic complexity to simulate alloy oxidation kinetics in relevant FE combustion (i.e., air- and oxy-fired) and working fluid (e.g., steam and sCO_2) environments. The primary focus will be on predicting long-term oxidation kinetics that would establish criteria for end of life in specific alloy systems. Doing so will allow either higher temperatures to be achieved for current systems at existing stress levels or higher stress levels within components at existing temperatures for current systems.



Multiscale-relay simulation of oxidation kinetics: Several essential physical processes in high temperature oxidation are incorporated into an integrated phase-field model, and through the novel multiscale-relay scheme based on the scaling feature of the phase-field model, the predicted oxidation kinetics coherently spans several orders of magnitude in length and time.

Materials Design and Development

Performer: NETL-ORD

Award Number: IPT_FY15 (tasks 3.1, 3.2 and 3.3)

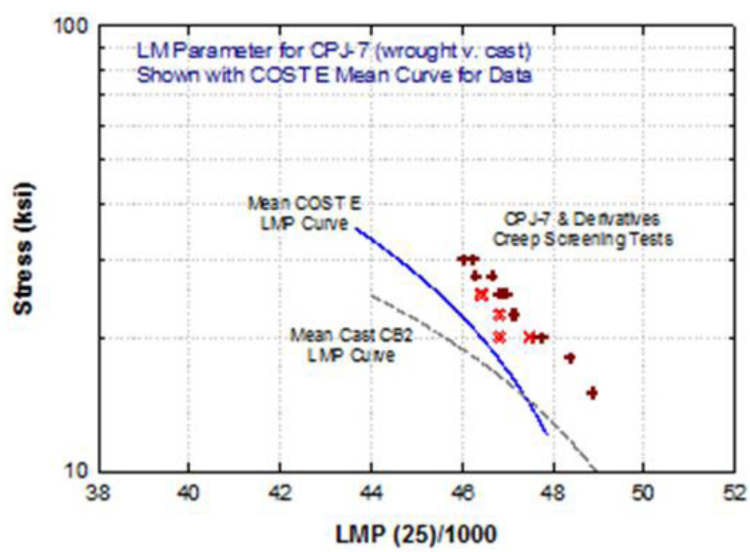
Project Duration: 10/1/2014 – 9/30/2015

Total Project Value: $500,000

Technology Area: Plant Optimization Technologies

In anticipating the Crosscutting Research Program need for new energy efficient and high temperature capable materials for constructions at conditions from USC to A-USC and beyond, such as materials of construction for components for sCO_2 cycles and advanced turbines, etc., and for providing material-ready solutions for the commercial sector, this project focuses on three materials research areas:

1. Advanced Martensitic-Ferritic Steels. This effort will build upon existing NETL research to further increase the service temperature (~5°C) and isothermal life (> 10%) of wrought and cast 9% Cr martensitic-ferritic steel for ultrasupercritical (USC), advanced ultrasupercritical (A-USC), and other high-temperature, harsh-environment applications.
2. Superalloy Design and Development. This research aims to improve high-temperature performance of both cast and wrought nickel-base superalloys through alloy design strategies (i.e., element and phase manipulation, heat treatment, and thermo-mechanical processing) and microstructure control (such as inducing twinning during processing, i.e., Twinning Induced Plasticity [TWIP]).
3. Advanced Fossil Energy Alloy Concepts. Researchers will assess, from a commercial manufacturing perspective, conditions for high-entropy alloy (HEA) manufacturing that delivers on the potential outstanding physical and mechanical properties of HEAs for use in FE applications. Benchmarks will be established for HEA microstructure and subsequent physical and mechanical properties through commercially relevant melting practices, and these will be compared to technically important commercial alloys (e.g., austenitic stainless steels).



Larson Miller Parameter plot for COST E & cast CB2 at temperatures from 1050 °F (565.5 °C) to 1200 °F (648.9 °C).

Advanced Alloy Design Concepts for High Temperature Fossil Energy Applications

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA114

Project Duration: 10/1/2013 – 9/30/2015

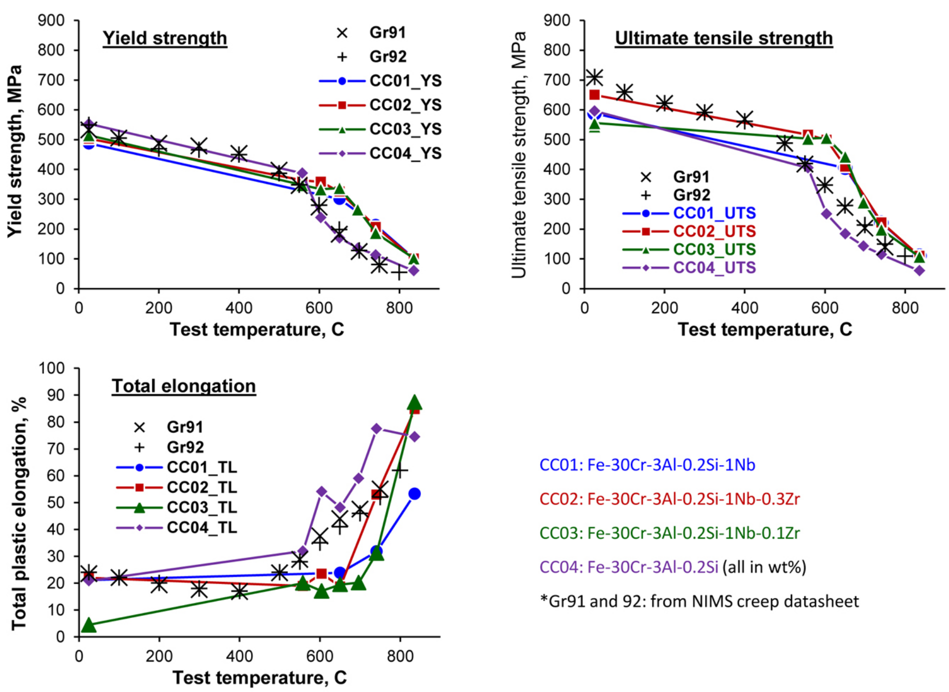
Total Project Value: $654,000

Technology Area: Plant Optimization Technologies

NETL is partnering with Oak Ridge National Laboratory 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 is 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 Technologies 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, to be 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.



Tensile properties of new high temperature alloys.

Corrosion Issues in Advanced Coal Fired Boilers

Performer: ORNL - Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA116

Project Duration: 10/1/2013 – 9/30/2015

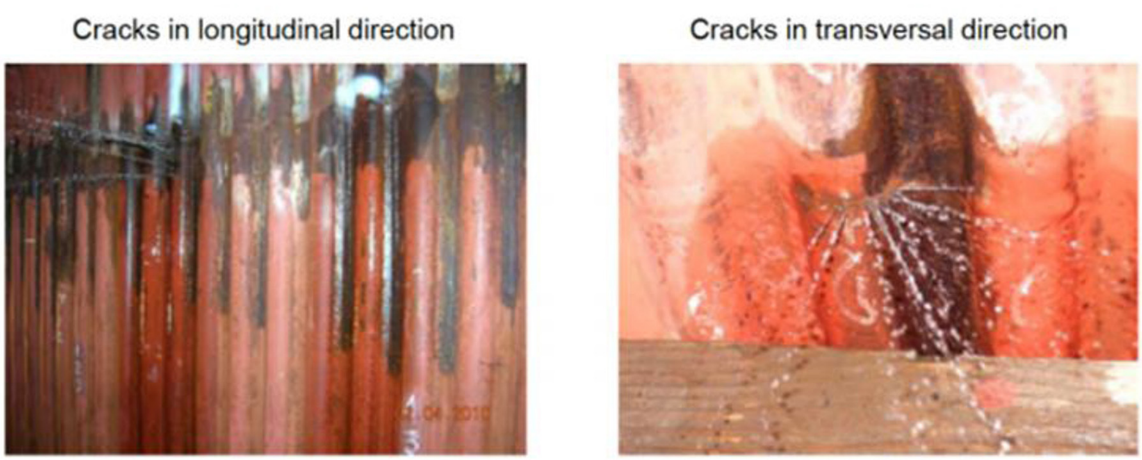
Total Project Value: $325,000

Technology Area: Plant Optimization Technologies

NETL is partnering with Oak Ridge National Laboratory to address critical corrosion and environmental effects issues in coal-fired boilers ranging from boiler water walls to super heater tubes. Specific technical objectives are to obtain better understanding of (1) hydrogen induced cracking in boiler water walls and which alloys that may be more resistant to this type of degradation and (2) the effect of shot peening on steam side oxidation of austenitic super heater tubes. Such understanding 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.

To achieve the project goal, this work will determine the temperature-relevant corrosion mechanisms; determine the role of environment on mechanical response; evaluate the upper temperature limit for new materials and surface modifications in terms of lifetimes; and characterize the reaction products and extent of alloy degradation under these conditions.

It is anticipated that the results will improve performance of commercial and model alloys in controlled laboratory experiments to simulate advanced fossil boiler conditions.



H-induced stress corrosion cracking.

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

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA115

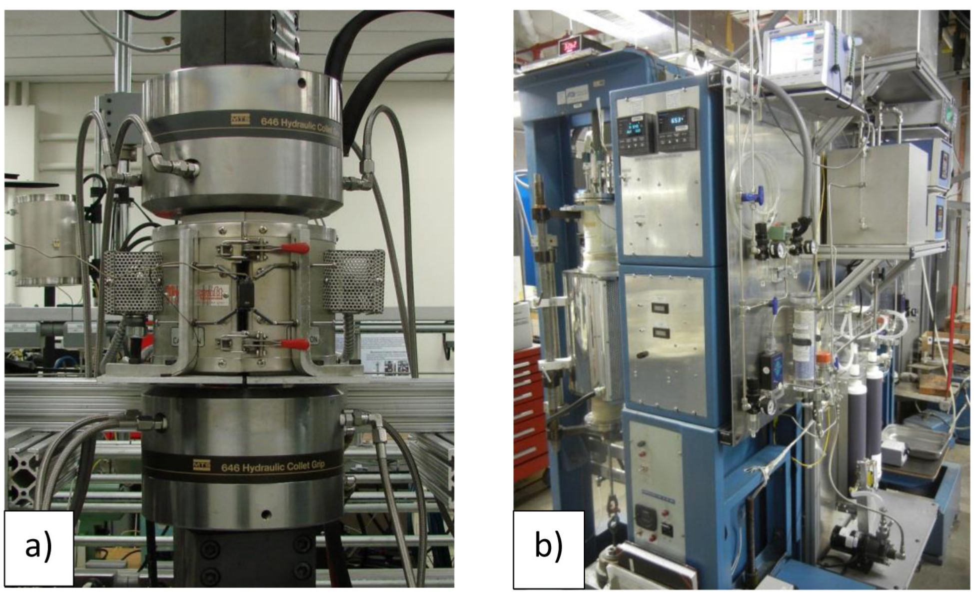
Project Duration: 10/1/2013 – 9/30/2015

Total Project Value: $670,000

Technology Area: Plant Optimization Technologies

NETL is partnering with Oak Ridge National Laboratory to generate pertinent creep-fatigue data and develop new lifetime models that will allow accurate prediction of the lifetimes of those fossil fuel power plant components that are subjected to flexible operation (e.g., load cycle following of renewable power generation). Such flexible operation can result in thermal-mechanical fatigue of components over long periods of time. The result can be premature failure of these components. Most existing coal fired power plants were not designed for this type of operation, and new advanced fossil fuel plants may need to include flexible operation in their thermal/mechanical design.

Improvements to creep-fatigue data and lifetime models will advance the development of advanced power plant designs to improvements in efficiency and operational flexibility and result in lower operating costs.



a) Servo-hydraulic creep-fatigue machine, b) Thermal cyclic creep machines allowing testing in steam.

Materials for Advanced Ultrasupercritical Steam Power Plants

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA061

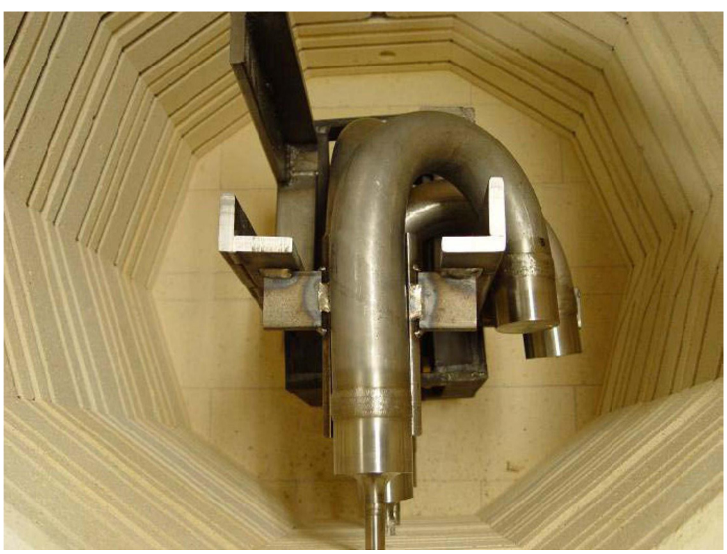
Project Duration: 9/29/2009 – 9/30/2015

Total Project Value: $2,329,000

Technology Area: Plant Optimization Technologies

NETL is partnering with Oak Ridge National Laboratory to assist with integration efforts into the overall U.S. DOE/OCDO sponsored Advanced Ultra-supercritical (AUSC) Steam Boiler Consortium activities which seeks to develop the materials technology required to operate a power steam boiler at steam conditions up to 7600C (14000F) and 350 bar (5000 psig) which will decrease emissions by up to 30% and reach efficiencies of up to 50%. Specifically, ORNL will continue its leadership of the Mechanical Properties task and its participation on the steam-side oxidation task. A new project to extend the work initiated in the original five-year program has been started by the AUSC Consortium (EPRI, EIO, four major U.S. boiler manufactures, and ORNL). For the Mechanical Properties task, ORNL will continue its work to evaluate the long-term behavior of the down-selected candidate alloys, investigate the effects of processing variables and welding, provide fundamental research needed in the areas of microstructural evolution at relatively long-times using electron microscopy and computational thermodynamics, and provide the necessary data to produce material models. The Steam-Side Oxidation task will focus on measuring oxidation kinetics pertinent to the range of conditions expected in USC steam boiler operation, and characterizing the evolution of scale morphologies to provide input on ultimate failure due to high oxidation rates or scale spallation. These data will be a major contribution to the database concerning environmental compatibility being assembled in the AUSC program.

The goal of this project is to develop the materials technology required to design, construct, and operate an AUSC steam boiler with reduced heat rate and increased efficiency. Scientific understanding of the effects of high temperatures and pressures on these advanced materials will provide a basis for the specification, design, fabrication, operation, and maintenance of AUSC steam power plants. The development of AUSC power plants will provide significant benefits in increased fuel efficiency and reduced carbon dioxide emissions, helping the U.S. to conserve fossil fuels and manage emissions.



Alloy 617 in cold.

Predicting the Oxidation/Corrosion Performance of Structural Alloys in Supercritical CO_2

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA334

Project Duration: 10/1/2014 – 9/30/2015

Total Project Value: $80,000

Technology Area: Coal Utilization Sciences

NETL is partnering with Oak Ridge National Laboratory (ORNL) on this project. The supercritical CO_2 (SCO_2) cycle at temperatures of 650 degrees Celsius and above has recently been proposed to provide breakthroughs in efficiency and CO_2 capture capability. To date, there is limited data on oxidation/corrosion in the SCO_2 cycle at these temperatures for structural alloys, and a model for predicting oxidation/corrosion rates and propensity for oxide exfoliation in supercritical CO_2 does not exist, hindering the material selection for these novel cycles. The ORNL effort will be focused on extending the exfoliation models already developed in collaboration with EPRI for steam oxidation/corrosion to those of supercritical CO_2 flows with impurities and applying them to the SCO_2 cycles. The oxidation and exfoliation will be modeled by developing sub-modules specific to the alloy(s) considered in this project. Numerical simulation results will be conducted for various supercritical CO_2 operational schedules in order to provide appropriate data on exfoliation tendency needed for the alloy selection.

The model developed will be a useful tool for power plant designers to select structural materials for various components in a supercritical CO_2 system, and for researchers to guide new alloy development work for supercritical CO_2 cycles.

Procured steel materials identified for testing.

Ultrasupercritical Steam Cycle Turbine Materials

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA069

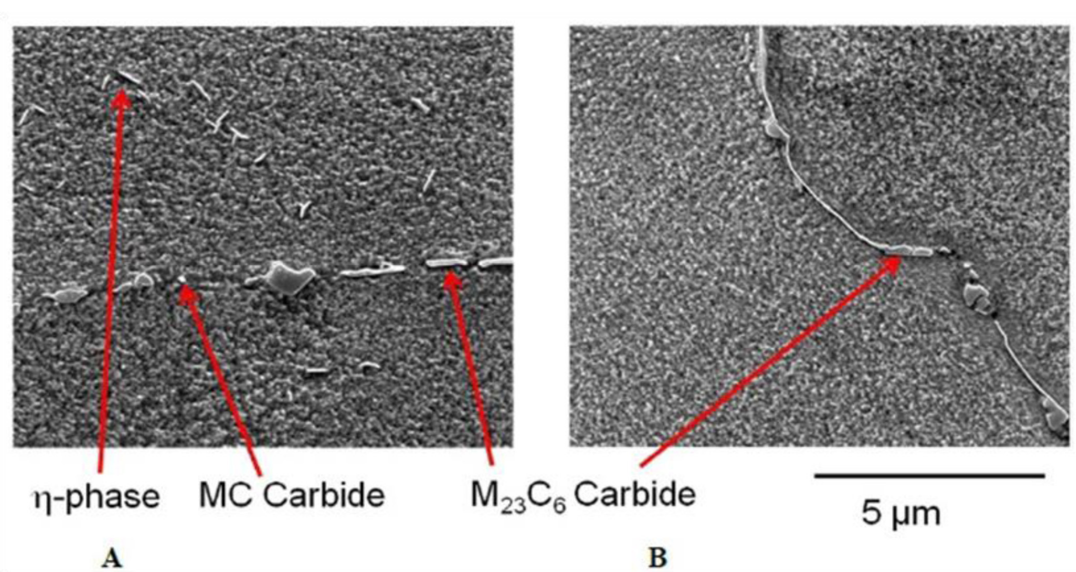
Project Duration: 10/1/2009 – 9/30/2015

Total Project Value: $2,250,000

Technology Area: Plant Optimization Technologies

NETL is collaborating with ORNL on a project to evaluate the behavior of high-temperature materials and contribute to defining the property requirements for steam turbine designs for operation under AUSC steam conditions. The project will use ORNL's expertise and facilities to develop methods for overcoming current materials limitations. The main areas of interest will be high-temperature creep strength, corrosion behavior in steam, and weldability. ORNL researchers will perform detailed evaluations to understand the potential for developing cast Ni-based alloys with improved strength and acceptable fabricability. Researchers will modify alloy compositions based on composition/structure/property interactions where improvements in performance in the cast turbine casing application are indicated.

The main objective of the project is to evaluate the behavior of high-temperature materials to complement the efforts of the U.S. USC Steam Turbine Consortium in defining property requirements for steam turbine designs for operation under AUSC steam conditions (760 °C and 345 bar/1,400 °F and 5,000 psig steam). This project will contribute advanced materials capable of extended operation at AUSC steam temperatures and pressures required for the next generation of highly efficient, low-emissions power plants. Such plants will improve the nation's ability to reduce greenhouse gas emissions and better solve issues associated with global climate change.



Scanning Electron Micrographs of cast and heat-treated microstructures of (A) a reference heat of Inconel 740 (formulation 2Nb-1.8Ti-0.9Al), and (B) new Inconel 740 (formulation 1.5Nb-1.5Ti-1.3Al), modified for improved weldability. Note the continuous carbide boundary film of B, which may be the cause of low creep rupture ductility. [Credit: NETL/Albany].

Weldability of Creep Resistant Alloys for Advanced Power Plants

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA118

Project Duration: 10/1/2013 – 9/30/2015

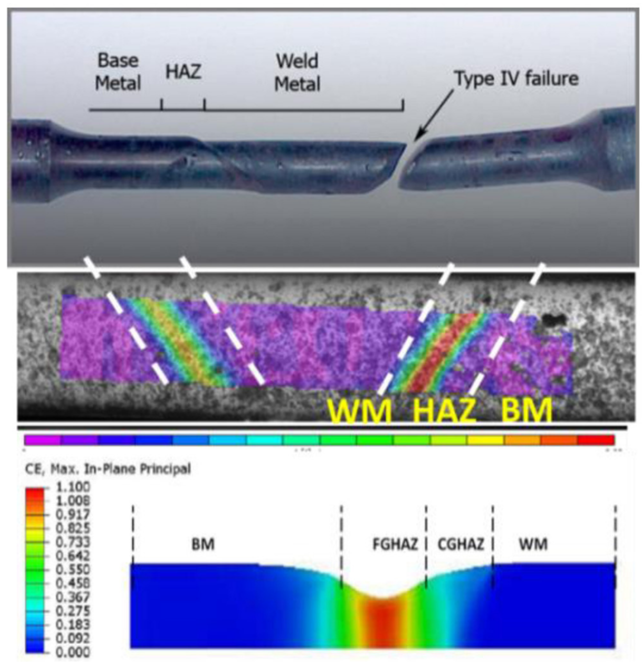
Total Project Value: $550,000

Technology Area: Plant Optimization Technologies

NETL is partnering with Oak Ridge National Laboratory on this project. This project aims to develop practical engineering solutions on two key issues on 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 state-of-the-art integrated computational welding mechanics modeling tool (ICWE) developed at ORNL; apply the integrated computational weld engineering (ICWE) modeling tool developed at ORNL 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; obtain the local creep and creep-fatigue constitutive behavior in different regions of a weld; and develop new welding and post heat treatment practices to improve the creep resistance of similar and dissimilar metal weldments.

The research will promote the development of advanced power plant designs that can operate at higher temperatures and pressures, leading to improvements in efficiency and operational flexibility and resulting in lower capital and operating costs.



(a) A crept sample showing Type IV failure in the HAZ of a cross-weld sample after 2500 hours of testing

(b) Full field creep strain measurement of Grade 91 steel cross-weld sample after 90 hours creep testing showing significant creep deformation localization in the HAZ that lead the HAZ failure. The measurement was by a specially developed digital image correlation technique at ORNL.

(c) Feasibility demonstration of ICWE modeling of creep strain localization in a cross-weld specimen after 13000 hours creep in this project.

Effective Exploration of New 760 Degrees Celsius-Capability Steels for Coal Energy

Performer: Ohio State University Research Foundation

Award Number: FE0008960

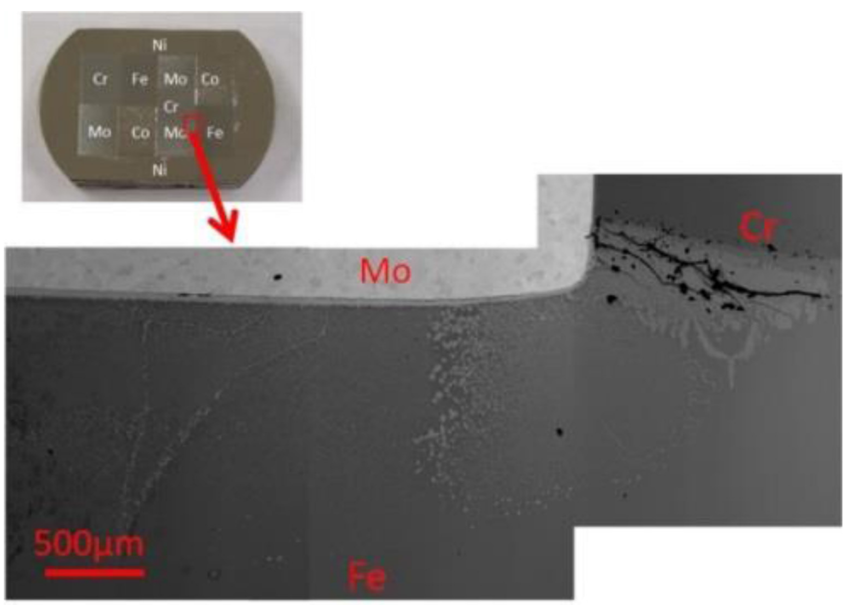
Project Duration: 9/1/2012 – 8/31/2015

Total Project Value: $299,934

Technology Area: University Training and Research

NETL is partnering with Ohio State University Research Foundation to perform research to develop new steels capable of operating at AUSC boiler and steam turbine conditions of approximately 760 degrees Celsius (°C) and 35 megapascals [1,400 degrees Fahrenheit (°F) and 5,000 pounds per square inch]. New compositions and new strengthening mechanisms or microstructures will be identified using computational thermodynamics and high-throughput diffusion multiples experiments. This method subjects a small sample of various metals to high temperature, thus creating many alloys, intermetallic compounds, and phases in one lab scale sample. The team will focus on exploring steel compositions with high iron and chromium concentrations. Specific objectives include (1) identifying at least one potent strengthening phase in ternary iron-chromium-molybdenum systems; (2) identifying and screening promising multi-component steel compositions for further tests; and (3) preparing samples of the two most promising multi-component steel compositions among those previously identified for further tests.

Project results will help improve the temperature capability of new steels in AUSC boilers and steam turbines, thus significantly reducing the cost of operating advanced coal-based energy generation systems. A successful outcome will provide the steel research community with a better understanding of strengthening phases that may be capable of operating at 760 °C and 35 megapascals for the typical lifetimes of coal fired power plants.



Montage image of an iron-chromium-molybdenum (Fe-Cr-Mo) triple region of a diffusion multiple that was dual-annealed at 1200 °C for 500 hours followed by 900 °C for 500 hours, showing several different precipitate phases with diverse sizes and morphologies.

Laves Phase-Strengthened Austenitic Steels for Coal-Fired Power Systems

Performer: Trustees of Dartmouth College

Award Number: FE0008857

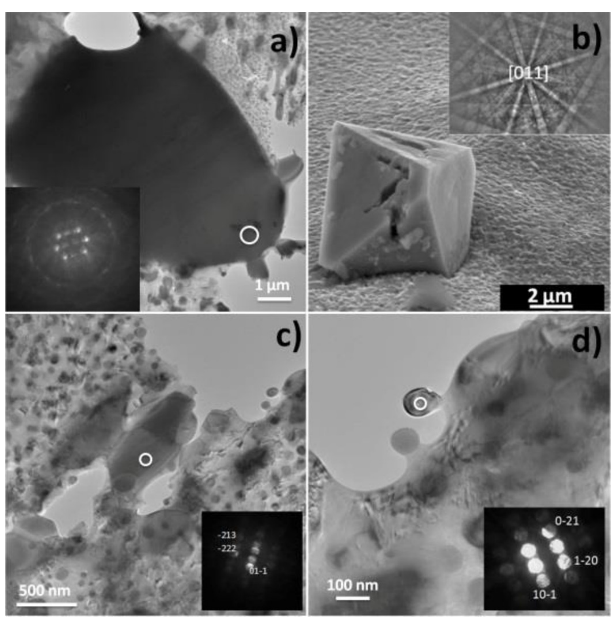
Project Duration: 9/1/2012 – 8/31/2015

Total Project Value: $402,467

Technology Area: University Training and Research

NETL is partnering with Dartmouth College to develop models of both precipitation kinetics and deformation behavior that can be used for further development of aluminum-alloyed Laves phase and L12-phase-strengthened austenitic steels. Specific objectives for the first year of the project include thermo-mechanical processing of fifteen specimens, microstructural analysis of the matrix and precipitates, and mechanical testing to determine room-temperature yield strengths and elongations in five specimens. Second-year objectives are thermo-mechanical processing of twenty specimens; microstructural analysis of particle size, spacing, precipitate chemistry, and tomography to select samples of interest in each state; mechanical testing to measure creep rates of microstructures, deformation analysis at various temperatures, and analysis of fracture behavior; and transmission electron microscopy (TEM) to analyze dislocation/precipitate interactions. Year three objectives include completing TEM in-situ annealing experiments, developing quantitative models to describe precipitation processes, and determining the relationship of microstructures to mechanical properties under various conditions.

Scientific insight into the effects of prior deformation on the precipitation processes and resultant mechanical properties of these advanced materials will provide a basis for the specification, design, fabrication, operation, and maintenance of advanced power generation plants. The development of advanced power plants will provide significant benefits in increased fuel efficiency and reduced carbon dioxide emissions, helping the U.S. to conserve fossil fuels and manage emissions.



SEM (b) and TEM (a, c, d) images of different precipitates in the thermo-mechanical treated aluminum-alloyed austenitic steels.

Serration Behavior of High-Entropy Alloys

Performer: University of Illinois

Collaborator(s): University of Tennessee

Award Number: FE0011194

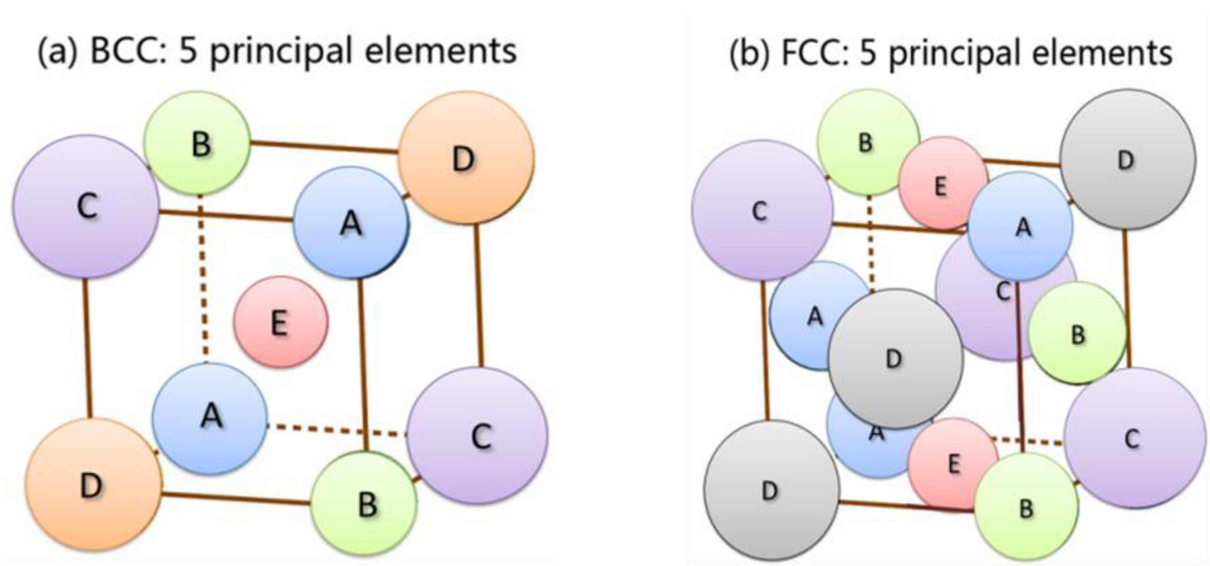
Project Duration: 10/1/2013 – 9/30/2016

Total Project Value: $300,000

Technology Area: University Training and Research

NETL is partnering with the University of Illinois to develop a novel statistical model that will be applied to the study of serration behaviors in high-entropy alloys (HEAs) under different conditions—a wide range of strain rates, temperatures, and compositions—as well as their compression and tension behaviors in order to elucidate the underlying mechanisms of plastic deformation in HEAs. The model will be used to predict fracture strength and creep life in these high-performance materials. The team will use predictions from statistical models to develop new materials-testing techniques and performance-prediction tools. Recent models predict that the size distribution of the serrations in the stress-strain curves at stresses that are far from failure provides the pertinent information about the failure (fracture) stress. The team will also study the long-term creep behavior of the alloys.

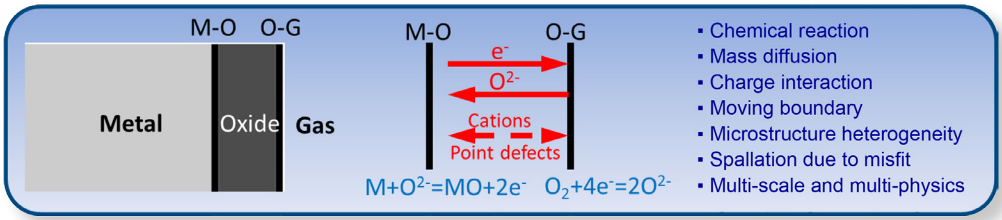
Computational modeling and simulation tools are needed to guide the design of new materials capable of operation under the extreme temperature, pressure, and corrosive conditions found in coal-fueled power plants. These tools will assist in decreasing the time and cost required to develop new materials compared to traditional trial-based methodologies.



(a) BCC: Body-Centered Cubic; (b) FCC: Face-Centered Cubic.

Computational Based Materials

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



Computational simulation of oxidation rate of high temperature alloys.

Computational and Experimental Development of Novel High-Temperature Alloys

Performer: Ames National Laboratory

Award Number: FWP-AL-07-360-019

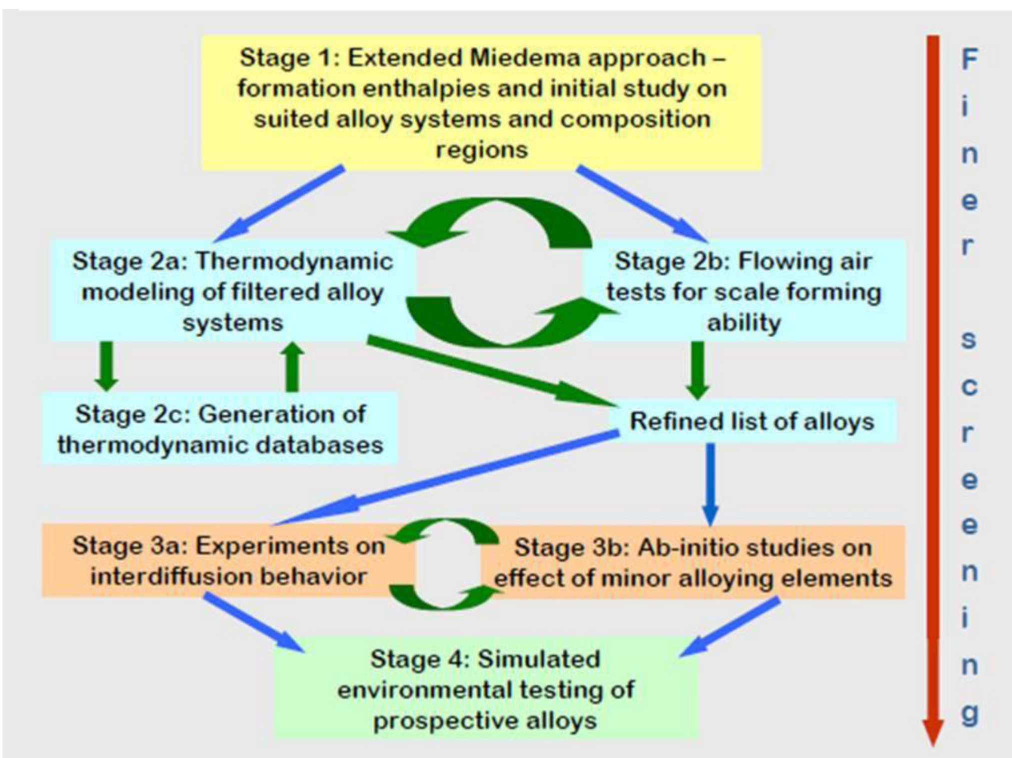
Project Duration: 10/1/2009 – 9/30/2015

Total Project Value: $575,000

Technology Area: Plant Optimization Technologies

NETL is partnering with Ames National Laboratory to develop a method for finding novel materials capable of performing well at very high temperatures required by advanced coal-fired power systems. This project will develop a tool to rapidly assess materials to find candidate high-temperature, oxidation-resistant alloys capable of meeting the requirements of high-temperature gas turbine components based on comparing formation enthalpy data of the materials. This tool will allow researchers to narrow possible alloy formulations from tens of thousands to a manageable number of combinations that are most likely to succeed. Project researchers will investigate potential alloy formulations using progressively more accurate thermodynamic methods, conduct critical experiments to test the accuracy of the calculations, and evaluate each alloy's key mechanical, thermal, and oxidation properties.

The goal of this project is to develop alloys capable of fulfilling the requirements stated in the FutureGen program using a multi-staged integrated methodology for systematically and efficiently searching multi- component metal alloy systems that have high melting points and good oxidation resistance at high operating temperatures. Promising alloys will then be screened for thermochemical stability using state of the art experimental methods.



Conceptual framework for alloy development process.

Computational System Dynamics (Computational Design of Multiscale Systems)

Performer: Ames National Laboratory

Award Number: FWP-AL-14-450-012

Project Duration: 10/1/2014 – 9/30/2015

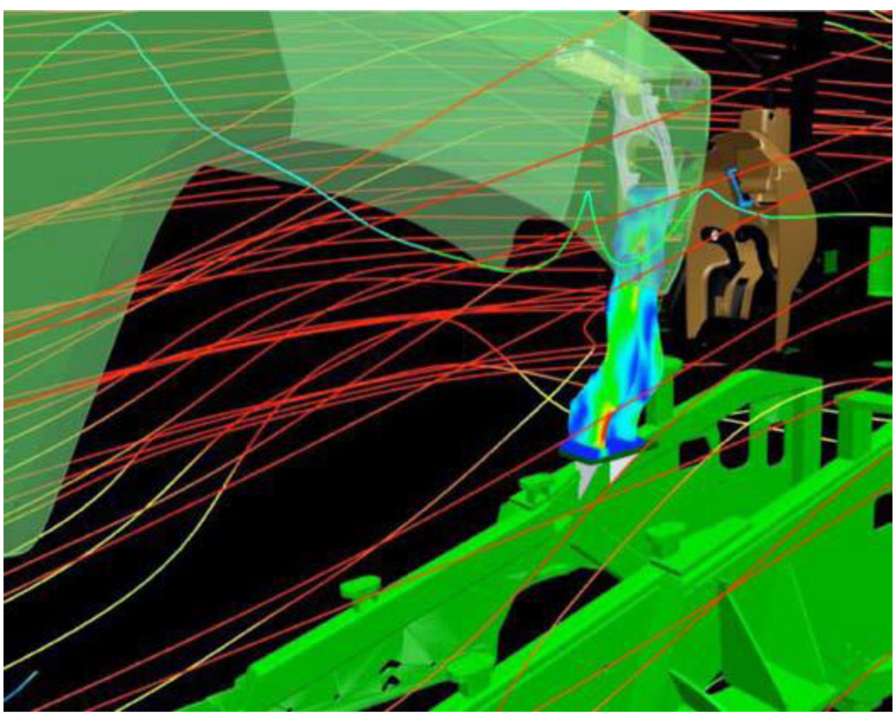
Total Project Value: $128,000

Technology Area: Coal Utilization Sciences

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

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

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



Graphic output from VE-suite of a simulation of the response of part of a part to an external load.

Modeling Creep-Fatigue-Environment Interactions in Steam Turbine Rotor Materials for Advanced Ultrasupercritical Coal Power Plants

Performer: General Electric Global Research

Collaborator(s): GE Energy, Massachusetts Institute of Technology

Award Number: FE0005859

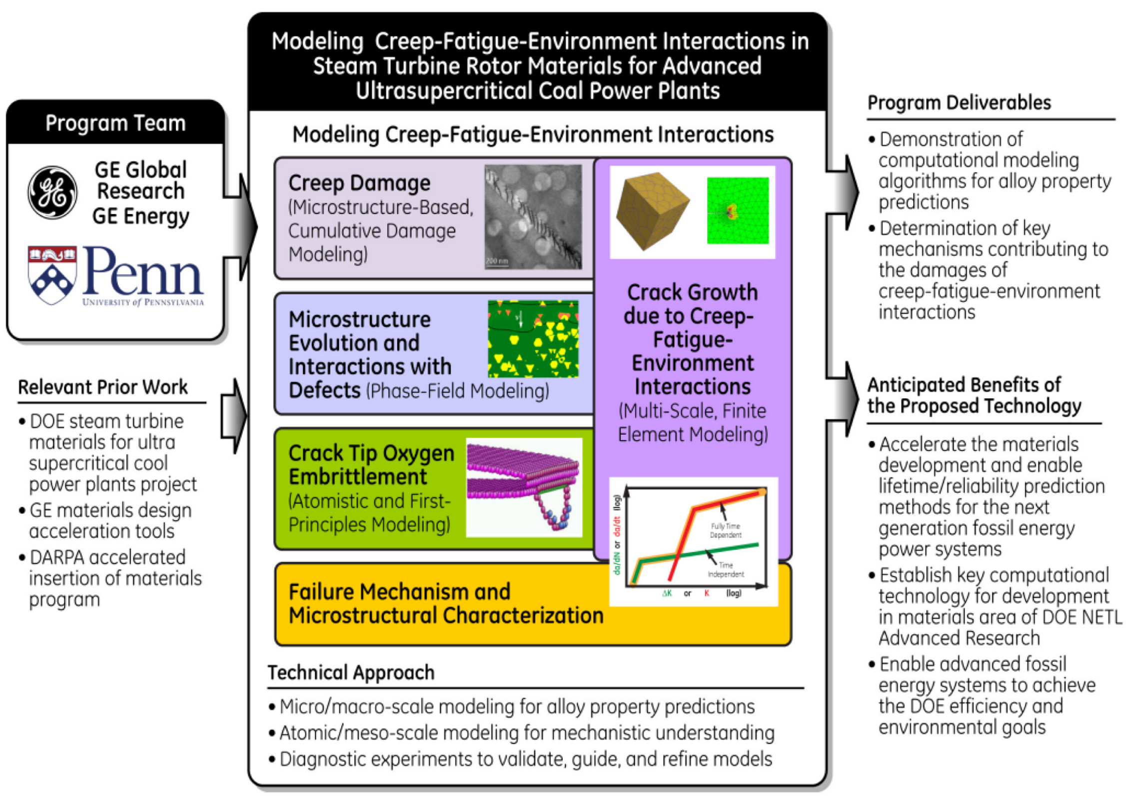
Project Duration: 1/21/2011 – 1/20/2014

Total Project Value: $1,499,928

Technology Area: Plant Optimization Technologies

NETL teamed with General Electric (GE) Global Research, GE Energy, and the University of Pennsylvania to address a very important aspect of materials design and service life prediction in future AUSC power plants: the creep-fatigue-environment interactions in steam turbine rotor materials. Despite the importance of creep-fatigue-environment interactions, they are not well understood. The project developed and demonstrated computational algorithms for alloy property predictions, and modeled key mechanisms that contribute to the damage caused by creep-fatigue-environment interactions. The project team built upon existing expertise, data, and materials modeling tools to develop multiscale (time and volume) computational algorithms and guidelines to understand and predict the chemical/mechanical response of nickel-based Haynes 282 superalloy to creep-fatigue-environment interactions at the temperature and pressure ranges expected in an AUSC steam turbine.

The results of this project include modeling creep-fatigue-environment interactions in steam turbine rotor materials for AUSC coal power plants, developing and demonstrating computational algorithms for alloy property predictions, and modeling key mechanisms that contribute to the damage caused by creep-fatigue-environment interactions. The methods developed in the project are expected to be applicable to other metal alloys in similar steam/oxidation environments.



Modeling Long-Term Creep Performance for Welded Nickel-Base Superalloy Structures for Power Generation Systems

Performer: General Electric Company

Award Number: FE0024027

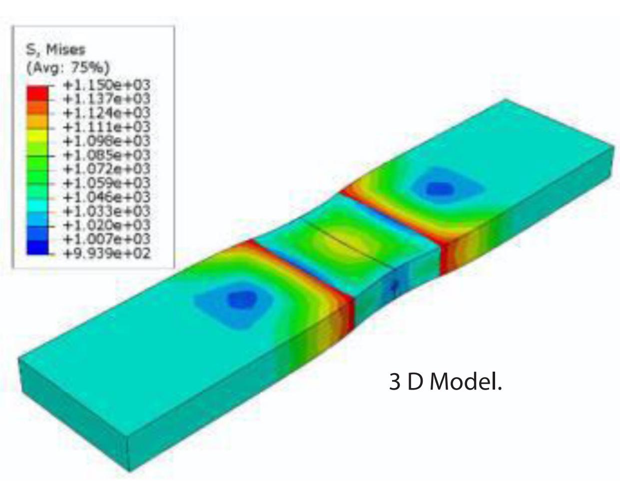
Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $649,707

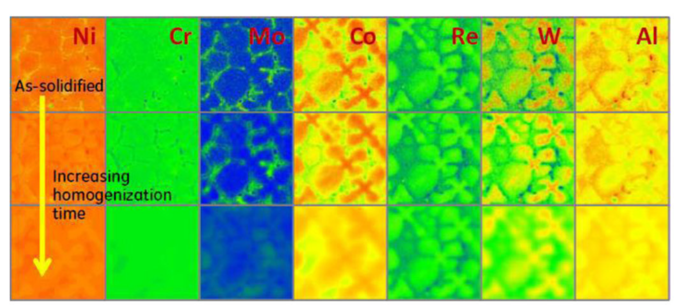
Technology Area: Coal Utilization Sciences

NETL is partnering with General Electric Company on this project to model long-term creep performance for nickel-base superalloy weldments in high temperature power generation systems. The project will use physics-based modeling methodologies and algorithms for predicting alloy properties in heterogeneous material structures. The modeling technology developed will provide a more efficient and accurate assessment of a material's long-term performance compared with current testing and extrapolation methods. This modeling technology will accelerate development and qualification of new materials in advanced power generation systems. The modeling methodology will be demonstrated on a gas turbine combustor liner weldment of Haynes 282 precipitate-strengthened nickel-base superalloy.

Results obtained from this project are expected to provide a better understanding of microstructural evolution in base material and welded H282 alloy in particular and wrought nickel-base alloys in general. This will help to predict performance of structural alloys subjected to high-temperature creep under realistic loading conditions of actual power generation components. While this work will be on gas turbine combustor liner application using a recently developed alloy, it will provide a general methodology for evaluating performance of new alloys for high-temperature applications. This approach is expected to reduce the time and cost to introduce new materials as well as the risk related to early failure due to microstructural changes during service.



3 D Model.



Multi-component and multiphase diffusion modeling.

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

Performer: Oregon State University

Award Number: FE0024065

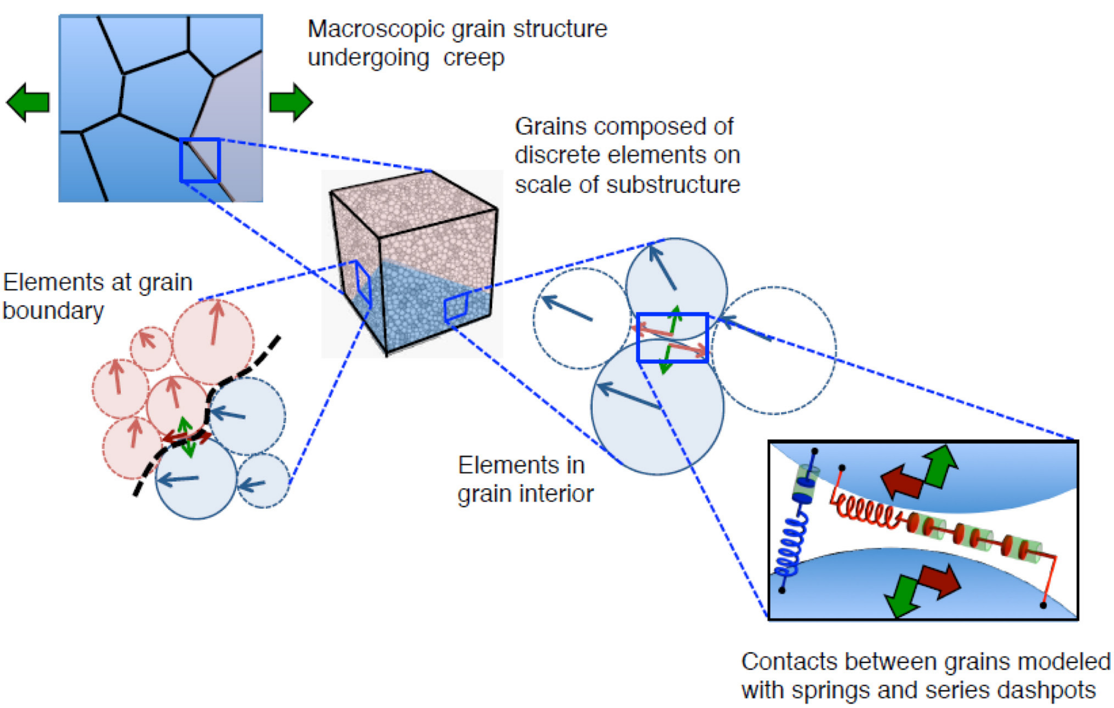
Project Duration: 1/1/2015 – 12/31/2016

Total Project Value: $624,999

Technology Area: University Training and Research

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

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



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

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

Performer: Pennsylvania State University

Award Number: FE0024056

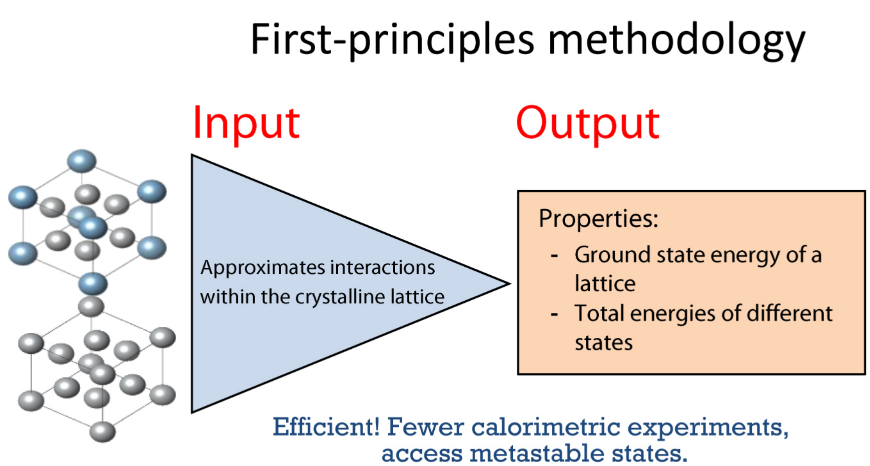
Project Duration: 1/1/2015 – 12/31/2016

Total Project Value: $632,176

Technology Area: University Training and Research

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

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



Shang et al. (2010) Computational Materials Science.

Predicting Microstructure-Creep Resistance Correlation in High Temperature Alloys Over Multiple Time Scales

Performer: Purdue University

Collaborator(s): University of California - San Diego

Award Number: FE0011291

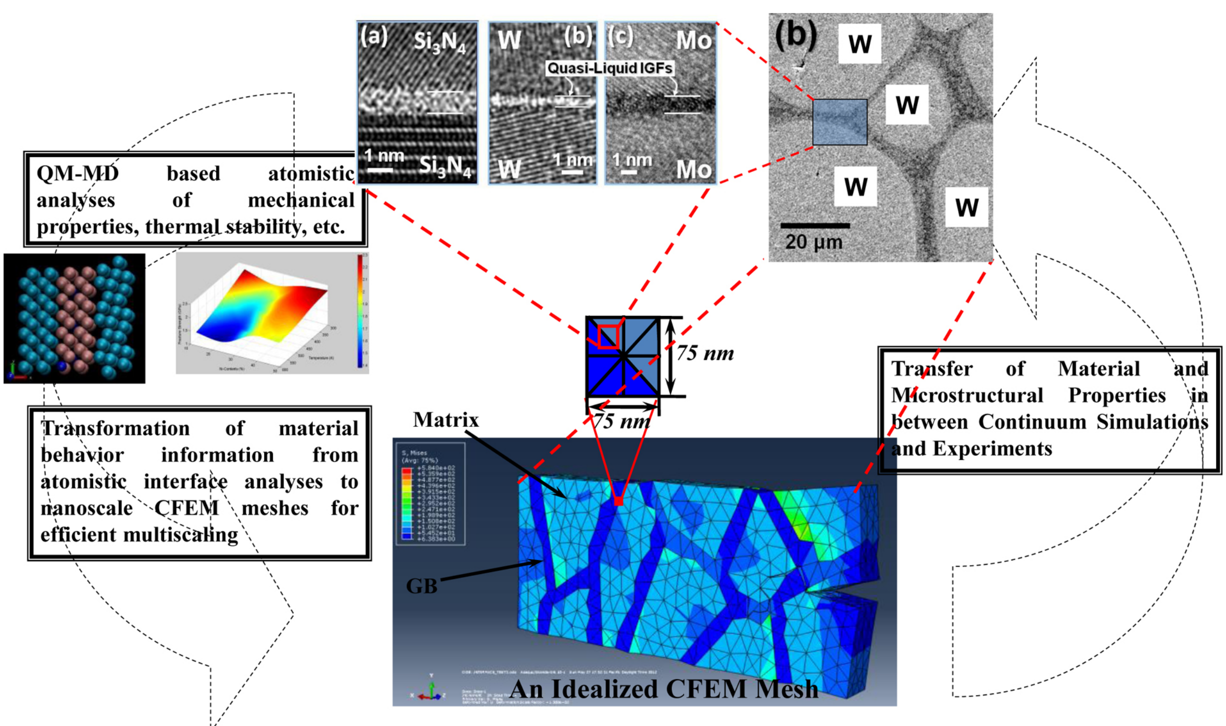
Project Duration: 7/22/2013 – 7/21/2016

Total Project Value: $300,000

Technology Area: University Training and Research

NETL is partnering with Purdue University to predict the creep and associated microstructure evolution of tungsten-based refractory alloys. Researchers will use grain boundary (GB) diagrams, a new concept, to establish time-dependent creep resistance and associated microstructure evolution of grain boundaries/intergranular films GB/IGF controlled creep as a function of load, environment, and temperature. The goal is to conduct a systematic study that includes the development of a theoretical framework, multiscale modeling, and experimental validation using W-based body-centered-cubic alloys, doped/alloyed with one or two of the following elements: nickel, palladium, cobalt, iron, and copper—typical refractory alloys. Prior work has already established and validated a basic theory for W-based binary and ternary alloys; the study conducted under this project will further extend this proven work.

Improvement to high-temperature advanced-materials will promote the development of advanced power plant designs that can operate at higher temperatures and pressures, leading to improvements in efficiency and operational flexibility and resulting in lower capital and operating costs.



Description of Multiscale Framework.

Computational Design of Weldable, High-Cr Ferritic Steel

Performer: QuesTek Innovations LLC

Award Number: SC0006222

Project Duration: 6/18/2011 – 8/7/2015

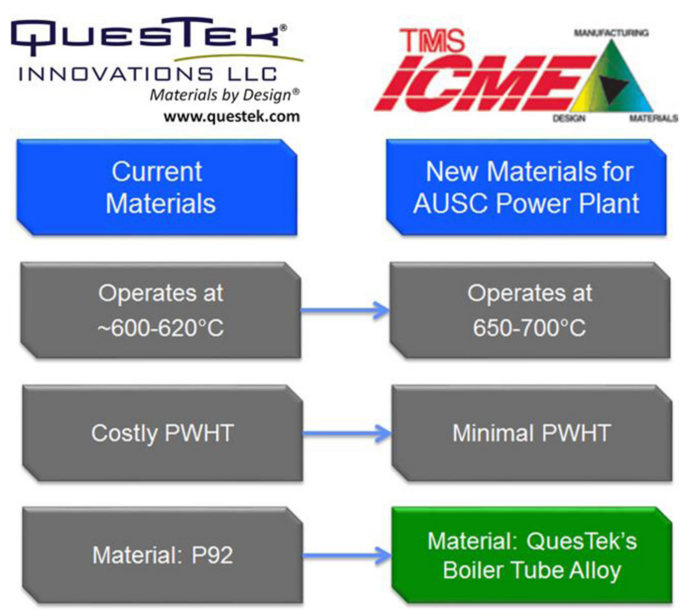
Total Project Value: $1,149,906

Technology Area: Plant Optimization Technologies

The U.S. Department of Energy (DOE) is actively funding research to significantly enhance the thermal efficiency of coal-fired steam boilers for power generation through the use of advanced ultra-super-critical (A-USC) steam temperatures and pressures. Since coal fired power plants are the dominant source of domestic power generation, the accelerated design, development and commercialization of efficient, reliable, next-generation coal-fired power plants can significantly increase domestic energy security and enhance the U.S. technical leadership strength.

The purpose of this SBIR program is to create a new alloy for A-USC coal-fired boilers using QuesTek's computational alloy design methodology and specific experience developing and commercializing a creep-resistant ferritic superalloy with low processing cost related to welding. During the Phase I program, QuesTek Innovations collaborated with engineers from a boiler OEM as well as technical experts from DOE to identify the elimination of post-weld heat treatment and increase in creep resistance as two critical material objectives for the new alloys. QuesTek then designed a series of prototype alloys using computational models to target critical design parameters, fabricated prototype samples for high-temperature tensile testing as well as welding demonstration. In Phase I, QuesTek's new alloys showed superb high temperature tensile strength and robust weld-zone microstructure unseen in incumbent alloys such as P92.

Based on the results from the Phase I prototype alloys and on input from project stakeholders, the objective of this Phase II project is to execute a detailed alloy design and demonstrate the performance and processing characteristics satisfying the alloy design criteria. Working with one of its suppliers, QuesTek will prototype ingots to specification at intermediate size scales (30 lb and 1,500 lb size). Alloy creep strength, weldability, and steam-side and fireside oxidation resistance will be demonstrated in the intermediate scale materials.



An Integrated Study on a Novel High Temperature High Entropy Alloy

Performer: Southern University and A&M College

Collaborator(s): Lawrence Berkeley National Laboratory - LBNL, Louisiana State University

Award Number: FE0011550

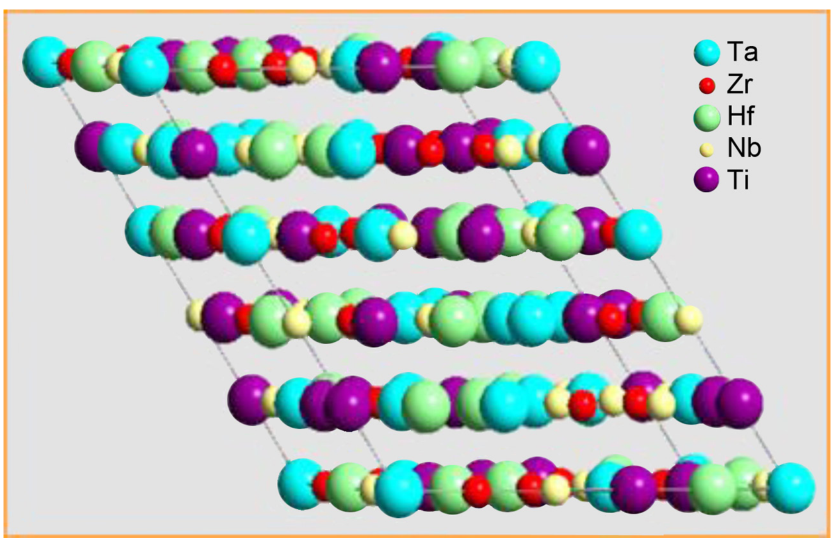
Project Duration: 10/1/2013 – 9/30/2015

Total Project Value: $200,000

Technology Area: University Training and Research

NETL is partnering with Southern University and A&M College to develop and experimentally validate a novel integrated method to improve the design of high entropy alloys (HEAs) for high-temperature and high-pressure gas turbine application. The project will also address the high-temperature and high-pressure oxidation resistance and low temperature ductility problems currently encountered in materials research for coal energy conversion. The project team will perform molecular dynamics (MD)/Monte Carlo (MC) simulation and interface that with energy high performance computing (HPC) simulation of the HEA models to screen out potentially high-temperature and high-pressure oxidation resistant and low-temperature ductile oxide dispersion strengthened (ODS) HEA candidates; perform experiments on the high-temperature and high-pressure property of the most promising ODS HEA systems from the simulation; and train students, integrating the materials design and HPC simulation into course work.

The research team will develop an understanding of the atomic-level processes that control high-temperature, high-pressure oxidation and low-temperature ductility performance of ODS HEAs. Additionally, participating HBCU students will receive training in the area of computation-based design of new materials.



A Body Centered Cubic (BCC) $Ta_{20}Nb_{20}Hf_{20}Zr_{20}Ti_{20}$ model: 100 atoms total, 20 atoms for each element. The blue balls are Ta, yellow balls are Nb, green balls are Hf, red balls are Zr, and purple balls are Ti.

Novel Nano-Size Oxide Dispersion Strengthened Steels Development Through Computational and Experimental Study

Performer: Southern University and A&M College

Award Number: FE0008382

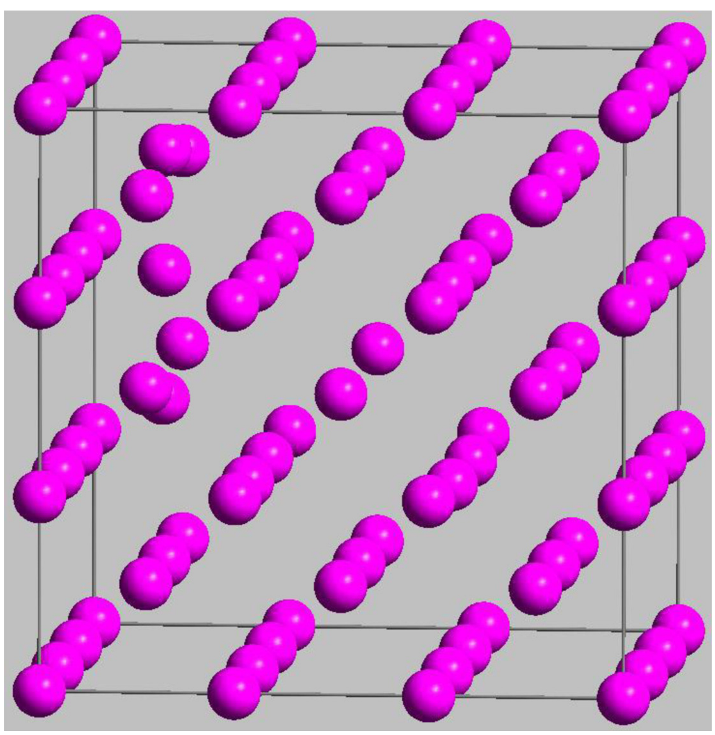
Project Duration: 6/1/2012 – 5/31/2015

Total Project Value: $200,000

Technology Area: University Training and Research

NETL is partnering with Southern University to use an integrated approach that combines computational materials design and experiments. These tools will simulate and determine key properties of new oxide dispersion strengthened (ODS) alloy compositions: elastic constants, interface bonding, dislocation creep, and microstructures at high-temperatures and applied stresses. The project team will (1) build interface models of ODS alloy compositions; (2) perform interface energy and molecular dynamics/Monte Carlo HPC simulations on the ODS alloy models to identify promising compositions for high-temperature and high-pressure applications; and (3) perform experiments to determine the high-temperature oxidation and high-temperature/high-pressure dislocation creep properties of the most promising ODS systems identified from the simulations.

The project team will identify improved ODS alloy compositions for high-temperature and high-pressure fossil energy applications and improved software codes for large-scale molecular dynamics simulations. Additionally, students from participating historically Black colleges and universities will receive training in the area of computation-based design of new materials.



Model of Nb Alloy for vacancy formation energy calculation.

Screening of Low Cost Ferritic Steels Designs for Advanced Ultra Supercritical Boiler Using First Principles Methods

Performer: Tennessee State University

Award Number: FE0011549

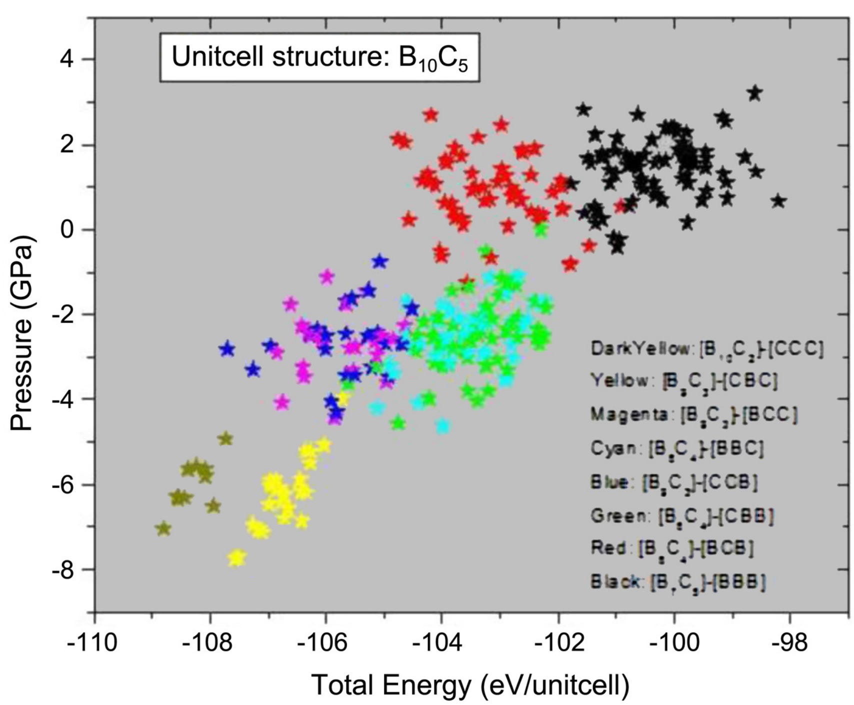
Project Duration: 9/1/2013 – 8/31/2015

Total Project Value: $200,000

Technology Area: University Training and Research

NETL is partnering with Tennessee State University to develop large scale screening approaches based on physical properties of matrix body-centered cubic solid solution phase of 9-12Cr ferritic steel. The goal of this project is twofold: (1) to extend a solid solution modeling module we developed in our current projects on Nb-Si based alloys to handle a larger number of elements, implement fast algorithms such as a special quasi-random structure method for physical properties calculation of solid solution, and develop modules to calculate additional properties need to assess ductility such as stack fault energy and surface cleavage energy; and (2) to calculate the Gibbs free energy and elastic properties of the BCC solid solutions for given composition sampling.

These methods are expected to have wide application in thermodynamic modeling of multi-component materials. It is expected that the results generated through the proposed research will provide valuable information that can be used to guide the design of ferritic steels which should speed the development of new ferritic steel with reduced creep rupture and corrosion for energy applications.



Local cluster configuration dependent energies of lattice with 1 unitcell type.

Synergistic Computational & Microstructural Design of Next-Generation High-Temperature Austenitic Steels

Performer: Texas Engineering Experiment Station

Award Number: FE0008719

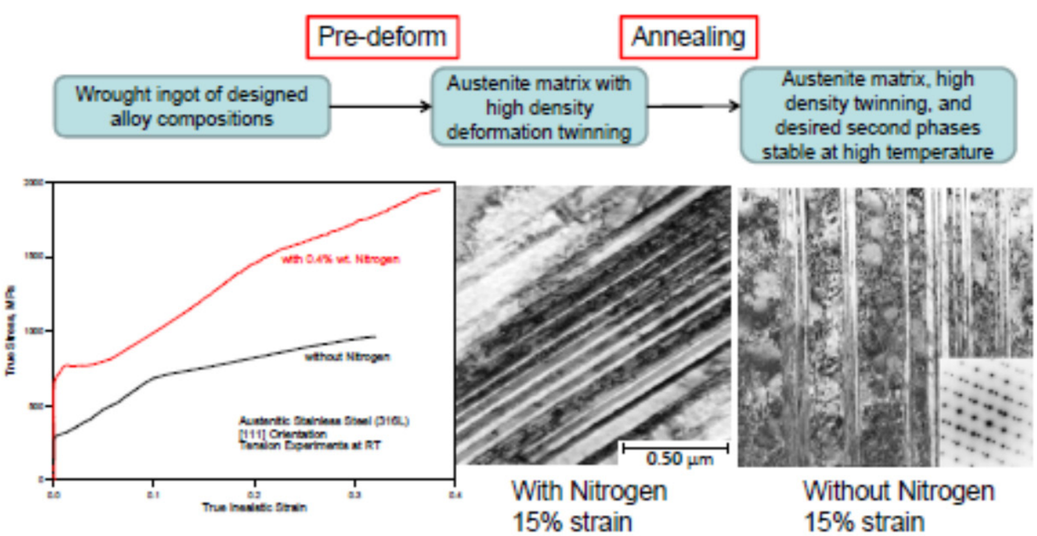
Project Duration: 8/1/2012 – 7/31/2015

Total Project Value: $300,000

Technology Area: University Training and Research

NETL is partnering with Texas Engineering Experiment Station to develop new austenitic stainless steels with ultrahigh strength, ductility, high temperature strength, and resistance to deformation and corrosion. Austenitic stainless steel is an allotrope of iron with alloying element(s), such as chromium and nickel. For this project, Texas Engineering Experiment Station will combine state-of-the-art computational and experimental alloy and microstructural design approaches to improve the high-temperature properties of austenitic stainless steels.

Effort will be devoted to create microstructures with homogeneously distributed nanoprecipitates (carbides, nitrides, carbonitrides, and intermetallics) formed at high temperatures (≥950 ºC), and intense density of low energy [high angle, low coincident side lattice] grain boundaries and crystal-twinning interfaces created through designed, simple thermo-mechanical processing pathways utilizing twinning-induced grain boundary engineering, and pinned by nano-precipitates. Both single-crystal and polycrystalline Ni-Cr grade austenitic stainless steels, with small additions of W, Nb, Mn, Cu, Al, Ti, N, and B, will be utilized to reveal the relation between the active deformation mechanisms, mechanical performance, and microstructure features such as twinning, crystallographic texture, and precipitates. After the new composition is created, thermo-mechanical processing and a twinning-induced grain boundary engineering route will be optimized for the desired microstructure. The resulting microstructure will be characterized as well as the high-temperature mechanical properties. A genetic algorithm approach is used as the major tool to optimize the micro-alloying, taking into account the low stacking fault energy, controlling of carbide/nitride formation, nano-size intermetallics, and the guideline from the preliminary foundation of the single-crystal stainless-steel study.



Simple thermo-mechanical processing.

Ab Initio Modeling of Thermomechanical Properties of Molybdenum-Based Alloys for Fossil Energy Conversion

Performer: University of Missouri – Kansas City

Award Number: FE0004007

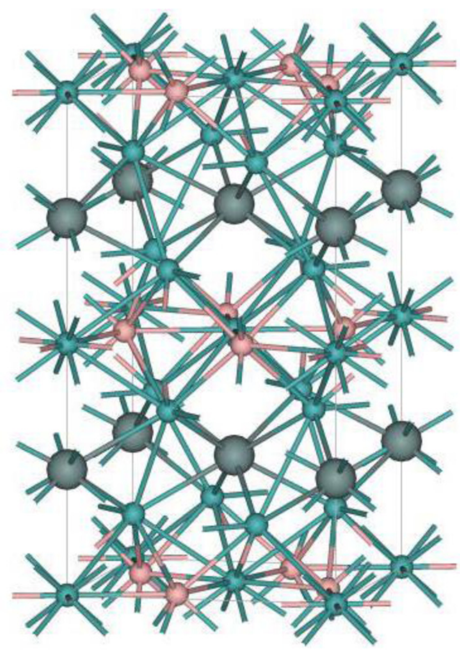
Project Duration: 7/1/2010 – 12/31/2013

Total Project Value: $299,925

Funding Source: University Training and Research

NETL has partnered with the University of Missouri–Kansas City in a project that will research and develop new molybdenum (Mo)-based materials for use in high-temperature, high-pressure environment applications in fossil energy conversion technologies. The project will also develop a new computational method and related algorithms to aid in modeling these new materials. This project will address this issue by targeting the development of computational tools required to design and optimize new non-ferritic based materials for this application.

The main goal of this project is to carry out extensive computational modeling on Mo-based composite alloys to identify those that can be used in high-temperature, high-pressure environments for applications in fossil energy conversion technologies. This project will make progress toward providing improved materials and computational modeling of these materials to support future implementation in fossil energy conversion technologies. These enhanced materials/alloys and a better understanding of their thermomechanical properties will enable a higher standard of fossil energy conversion to be realized, which will provide an overall higher energy output.



Mo_5SiB_2 crystal in tetragonal cell.

Large Scale Simulations of the Mechanical Properties of Layered Transition Metal Ternary Compounds for FE Power Systems

Performer: University of Missouri – Kansas City

Award Number: FE0005865

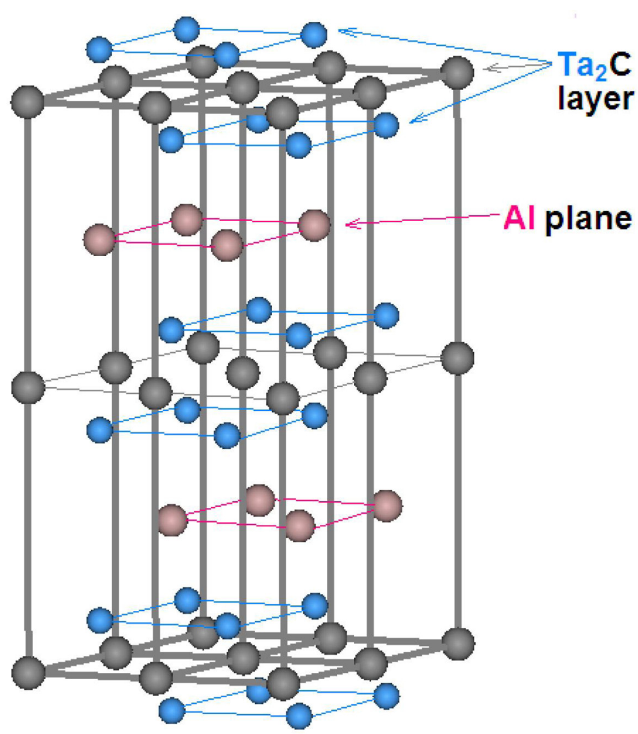
Project Duration: 8/1/2010 – 12/31/2014

Total Project Value: $1,127,346

Technology Area: Coal Utilization Sciences

NETL teamed with University of Missouri–Kansas City and Tennessee State University to conduct computational studies supporting the search for novel materials that can meet requirements of AUSC systems. This project focused on the computational development of a new class of materials called MAX phases, or $M_{n+1}AX_n$ [M = a transition metal, A = aluminum (Al), X = carbon (C) or nitrogen (N)]. The MAX phases are layered transition metal carbides or nitrides having the rare combination of metallic and ceramic properties. Due to their unique structural arrangements and directional bonding (both covalent and ionic), these thermodynamically stable alloys possess desirable properties such as damage resistance, oxidation resistance, excellent thermal and electric conductivity, machinability, and fully reversible dislocation-based deformation.

The project goal was to predict and understand the mechanical properties of the MAX phase compounds for potential application in extreme high-temperature, high-pressure, and highly corrosive environments. These new computational methods and algorithms have advanced the search for novel materials that can meet evolving requirements without incurring costly trial-and-error laboratory tests.



Ball and Stick Model of typical MAX Phase (Ta_2AlC) showing the layered structure in a 2x2x1 supercell.

Computational Microstructural Optimization Design Tool for High Temperature Structural Materials

Performer: University of North Texas

Award Number: FE0008648

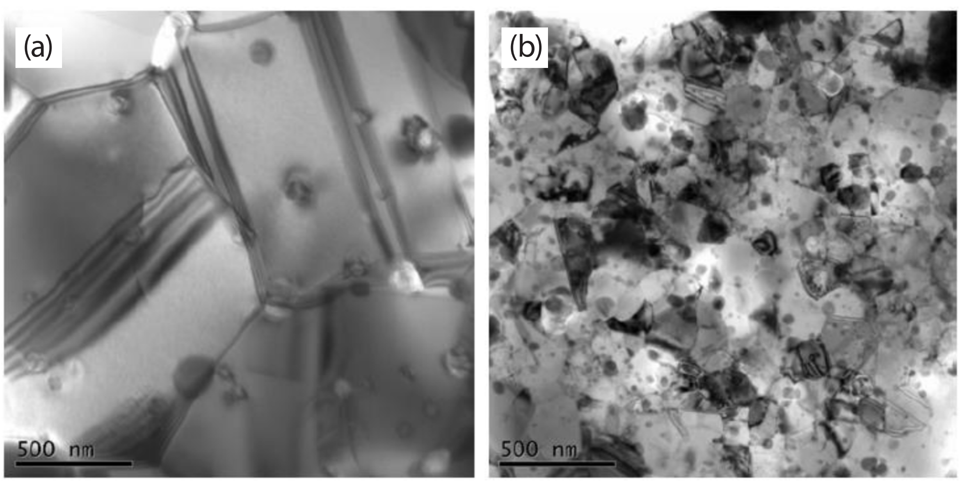
Project Duration: 9/1/2012 – 2/28/2015

Total Project Value: $300,000

Technology Area: University Training and Research

NETL partnered with the University of North Texas to develop a Ni-Cr based high performance alloy. The nano-composite Ni-20Cr is aimed at high-temperature structures that require a combination of high stiffness and high creep strength in an oxygen-rich and hydrogen-rich high-pressure environment. The objectives of the research project were twofold: (a) develop a methodology for microstructural optimization of alloys, a genetic algorithm approach for alloy microstructural optimization using theoretical models based on fundamental micro-mechanisms, and (b) develop a new computationally designed Ni-Cr alloy for coal-fired power plant applications. The project was successful on both goals.

This new approach—development of materials by design rather than by discovery—has the potential to significantly reduce the cost and time for development of high-performance engineered materials.



TEM bright field images of SPSed (a) Ni-20Cr and (b) Ni-20Cr-1.2Y2O3 alloys.

Computational Design and Performance Prediction of Creep-Resistant Ferritic Superalloys

Performer: University of Tennessee

Award Number: FE0024054

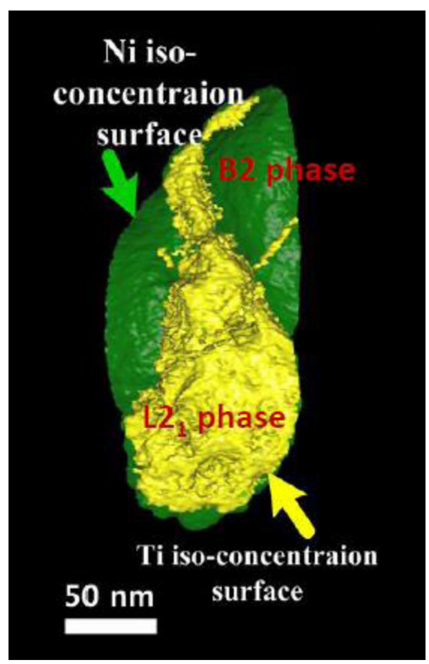
Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $626,681

Technology Area: University Training and Research

NETL is partnering with University of Tennessee on this project, the objectives of which are (1) to develop and integrate modern computational tools and algorithms, i.e., predictive first-principles calculations, computational-thermodynamic modeling, and meso-scale dislocation-dynamics simulations, toward design of high-temperature alloys for applications in FE power plants; and (2) to understand the processing-microstructure-property-performance links underlying the creep behavior of novel ferritic alloys strengthened by hierarchical coherent B2/L21 precipitates.

The proposed research will advance computational modeling used in the accelerated design of high-temperature alloys. The methods developed to compute thermodynamic and kinetic quantities from first-principles calculations will be applicable to other alloy systems. Quantitative creep modeling will lay a foundation for designing a wide range of advanced precipitation-strengthened alloys. It is also expected that the project will develop a novel creep-resistant hierarchical ferritic superalloy for applications in advanced steam-turbine systems and will train Ph.D. students and research associates in the integration of state-of-the-art computational and experimental methods that will form the framework for modern alloy design.



Courtesy of Center for Nano-phase Materials Sciences at ORNL (DOE) - G. Song, Z. Sun, P. K. Liaw, Unpublished, UTK.

Computational Design of Creep-Resistant Alloys and Experimental Validation in Ferritic Superalloys

Performer: University of Tennessee

Collaborator(s): Northwestern University; University of California, Berkeley

Award Number: FE0005868

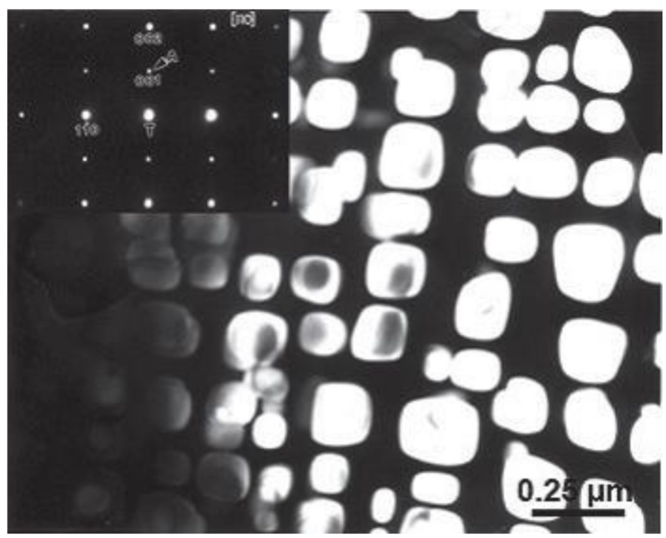
Project Duration: 10/1/2011 – 12/31/2014

Total Project Value: $1,533,680

Technology Area: Plant Optimization Technologies

NETL worked with the University of Tennessee, Northwestern University, and the University of California, Berkeley on advancing computational capabilities for the development of materials for next generation fossil energy power systems. The elevated temperatures required in USC steam turbines create a critical concern related to the creep strength of current ferritic steels. This project addressed this concern by targeting the development of computational tools required to design and optimize ferritic superalloys. These tools were used to measure microstructural characteristics of selected alloys to quantify the links among materials processing, microstructure, material properties, and performance. The information generated through utilizing these tools allowed researchers to gain an understanding of the creep behavior of these high-temperature alloys.

The goal of this project was to develop computational tools required to design and optimize ferritic superalloys needed for fossil-energy power plants operating at advanced steam turbine operating conditions. This project facilitated progress toward improved materials and computational modeling of these materials for use in fossil energy conversion technologies. These enhanced ferritic alloys and a better understanding of their creep behavior will enable a higher standard of fossil energy conversion, which will provide an overall higher energy output.



Dispersion of B2-NiAl-type precipitates in a bcc-Fe matrix (G. Ghosh, unpublished research, NU).

Experimental and Computational Investigation of High Entropy Alloys for Elevated High Temperature Applications

Performer: University of Tennessee

Collaborator(s): Computherm LLC

Award Number: FE0008855

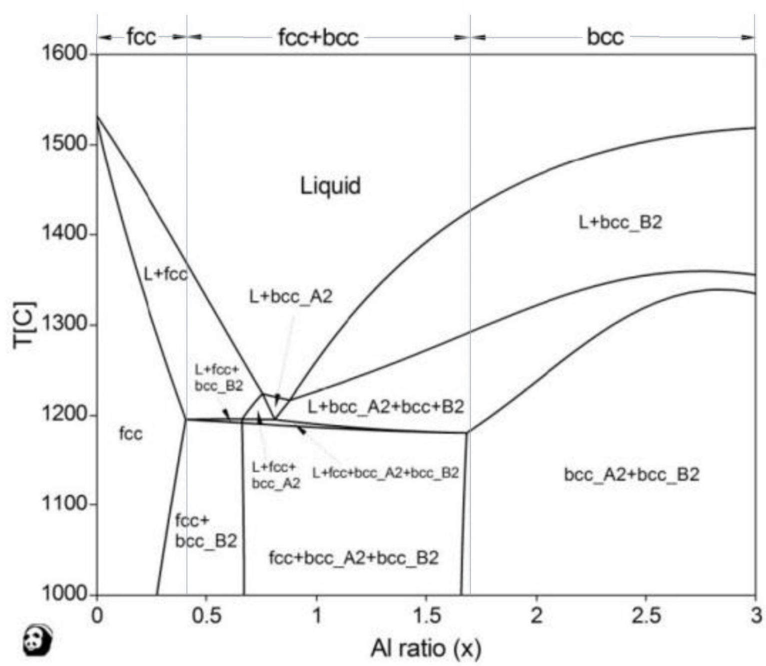
Project Duration: 8/1/2012 – 7/31/2015

Total Project Value: $300,000

Technology Area: University Training and Research

NETL is partnering with University of Tennessee to identify and develop high-entropy alloys (HEAs) that have key mechanical properties for use at elevated temperatures. Project personnel will make samples of the desired HEA compositions and perform compositional and microstructural analyses to characterize the structures of the developed HEAs. Researchers will perform conventional room-temperature and elevated-temperature uniaxial tensile and creep experiments. They will also use advanced characterization techniques, such as neutron and synchrotron diffraction, to determine structural changes of the new HEAs under applied stresses at high temperatures. The objectives of this project are to (1) perform fundamental studies on the Al_xCrCuFeMnNi HEA system to determine its potential for use in AUSC boilers and steam turbines at 760 °C and 35 Megapascals (MPa) and higher, and (2) develop an integrated approach to coupling thermodynamic calculations and focused experiments to identify HEAs that outperform conventional alloys.

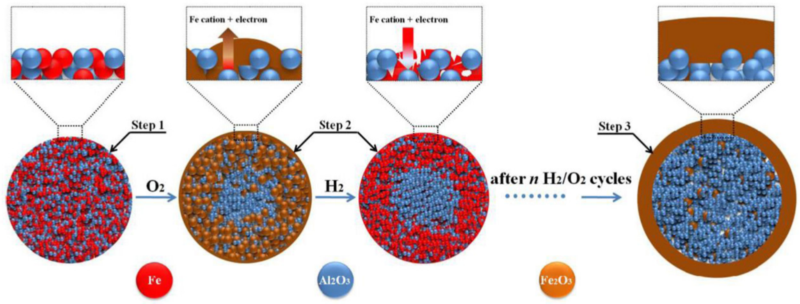
The expected results of the project will be one or more new HEA compositions that have the required mechanical properties (ductility and creep strength) to function in AUSC boilers up to 760 °C and a steam pressure of 35 MPa. The results will also demonstrate a computer-aided design approach for identifying and developing new types of alloys for advanced high-temperature fossil energy applications.



Calculated isopleth of the Al_xCoCrCuFeNi HEA system using thermodynamic descriptions. Similar calculations will be performed for the Al_xCrCuFeMnNi HEA system to assist in the design of HEAs suitable for use in high-temperature applications.

Functional Materials

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



Oxidation and reduction cycles: ionic diffusion.

Performer	Project Title	Page
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Gas Turbine Materials Life Assessment and Non-Destructive Evaluation

Performer: Argonne National Laboratory (ANL)

Collaborator(s): Siemens

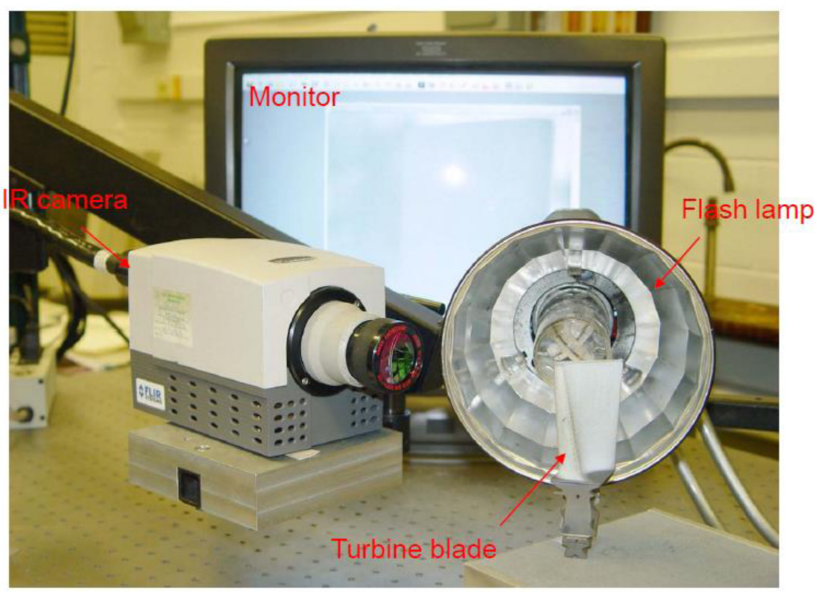
Award Number: FWP 49022

Project Duration: 10/1/2015 – 9/30/2017

Total Project Value: $260,000

Technology Area: Plant Optimization Technologies

NETL is partnering with Argonne National Laboratory for development and demonstration of advanced non-destructive evaluation inspection tools and technologies for hot gas path components to enable ongoing assessment of the remaining lives of components during their use. The goal of this project is to develop and demonstrate an in-situ flash thermography system for life prediction in gas turbines. The project will develop predictive models for deposition, corrosion, and component life assessment in gas turbines operating on novel fossil fuel gases. It is expected also that this work will develop and demonstrate advanced NDE inspection tools and technologies for hot gas path components to enable ongoing assessment of the remaining lives of components during their use. This work will allow for development and improvement of advanced materials technologies and may lead to maximization of power plant efficiencies while minimizing CO_2 emissions.



One-sided Flash Thermal Imaging Setup for testing TBC-Coated Turbine Blade.

Reduced Cost Bond Layers for Multi-Layer Thermal/Environmental Barrier Coatings

Performer: Auburn University

Collaborator(s): Plasma Processes Inc.

Award Number: FE0011245

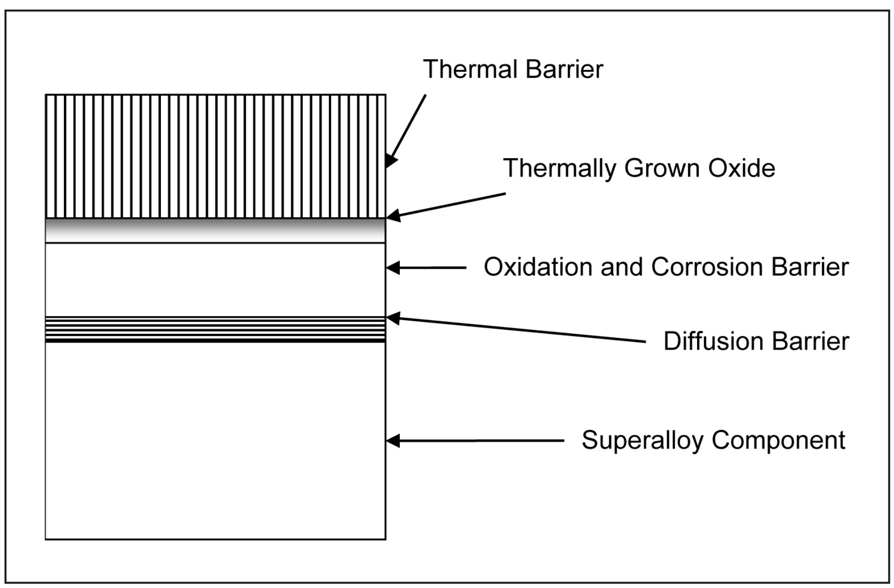
Project Duration: 7/17/2013 – 7/16/2016

Total Project Value: $362,310

Technology Area: University Training and Research

NETL is partnering with Auburn University to develop and investigate the degradation of a thermal barrier coating (TBC)/environmental barrier coating (EBC) system. The project involves the development of a TBC/EBC coating system and investigation of the degradation of the coating system. The focus of the project is on the interlayer between the alloy and ceramics TBC and the hot corrosion behavior of prospective lanthanide zirconate pyrochlore (a complex oxide mineral composed of niobium, sodium, and calcium that forms brown to black, glassy octahedral crystals and irregular masses) materials. In particular, the interaction of the outer pyrochlore layer with a calcium-magnesium-alumino-silicates deposit and different gas atmospheres is being evaluated.

The development of these technologies will reduce the cost and increase the efficiency of power-generation facilities with carbon capture in eight specific pathways: sensors, controls, and novel concepts; dynamic modeling; high-performance materials and modeling; water-emissions management and controls; carbon capture simulation; carbon storage risk assessment; innovative energy concepts; and systems analyses and product integration.



Proposed thermal protection architecture.

Advanced Thermal Barrier Coatings for Next Generation Gas Turbine Engines Fueled by Coal-Derived Syngas

Performer: Brown University

Award Number: FE0008933

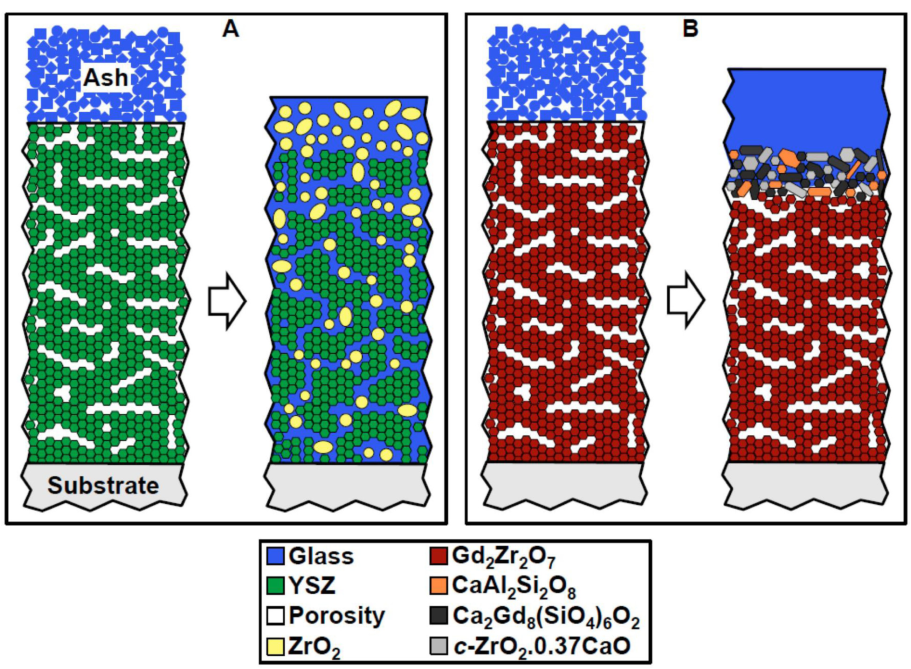
Project Duration: 9/1/2012 – 8/31/2015

Total Project Value: $324,400

Technology Area: University Training and Research

NETL is partnering with Brown University to fabricate and characterize optimized two-layer 48YSZ/7YSZ TBCs on bond-coated superalloy substrates. Researchers will measure the mechanical and thermal properties of the new TBCs and investigate the high-temperature interactions between lignite coal fly ash and the new TBCs at high temperatures (isothermal conditions). This will be followed by an investigation into the thermal cycling behavior of new TBCs under thermal gradient conditions with spray of lignite coal fly ash and water. Researchers will then model the thermo-chemomechanical failure and durability of the new TBCs tested under those conditions. Finally, the new TBC technology with optimized compositions and microstructures will be transferred to equipment manufacturers for further development and possible utilization in IGCC syngas-fired turbine engines. The overall goal of this research is to elucidate the feasibility of two-layer air plasma-sprayed TBCs for next generation IGCC syngas-fired turbine engines. These engines will operate at higher temperatures and in more hostile environments than currently available turbines. In support of the overall goal, the new coatings will exhibit (1) high-temperature capability, (2) low thermal conductivity, (3) resistance to attack by molten silicate (coal fly ash) deposits, (4) resistance to degradation by high moisture, (5) high durability, (6) improved manufacturability, and (7) low cost.

Successful results from this project will have a positive impact on gas-turbine engines, including improved durability and reliability, reduced maintenance, fuel flexibility, and lower cost. In addition, this project will result in the training of one graduate student for the future workforce.



Schematic diagrams of APS TBCs cross-sections with lignite fly ash deposits, before and after exposure to heat, depicting the interactions: (A) 7YSZ and (B) $Gd_2Zr_2O_7$. Diagrams not to scale.

Engineering Accessible Adsorption Sites in Metal Organic Frameworks for CO_2 Capture

Performer: Clark Atlanta University

Award Number: FE0022952

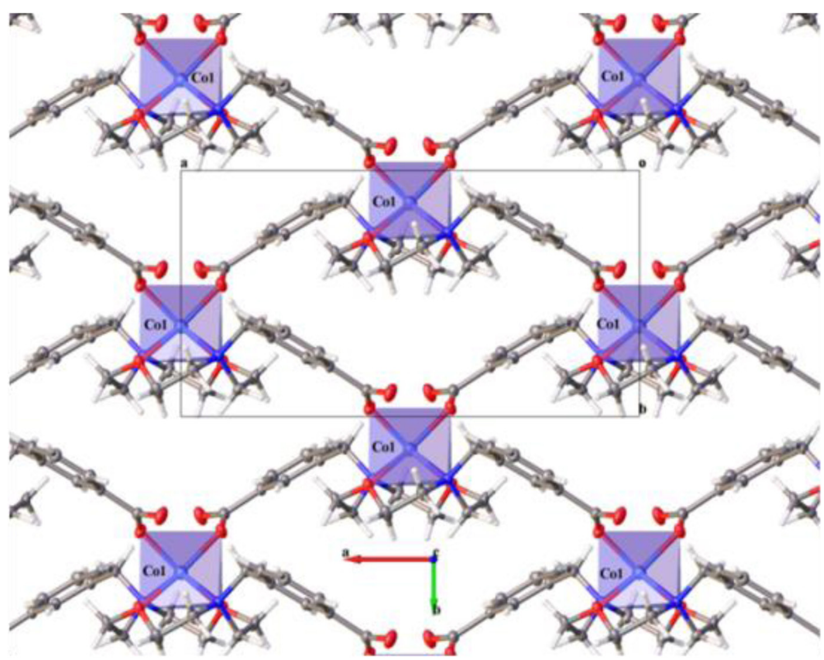
Project Duration: 10/1/2014 – 9/30/2017

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 CO_2 adsorption and selectivity properties. CAU will synthesize and characterize ultra-high-surface-area metal organic framework (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 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 (PXRD), 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 (DOE) 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 towards producing advanced sorbents for for CO_2 capture. Successful CO_2 adsorbent materials have the potential to have an industrial and environmental impact. This project will also provide research opportunities for students in the fields of chemistry, materials, and science related to the use of fossil energy resources.



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

Novel Silica Nanostructured Platforms with Engineered Surface Functionality and Spherical Morphology for Low-Cost High-Efficiency Carbon Capture

Performer: Delaware State University

Award Number: FE0023541

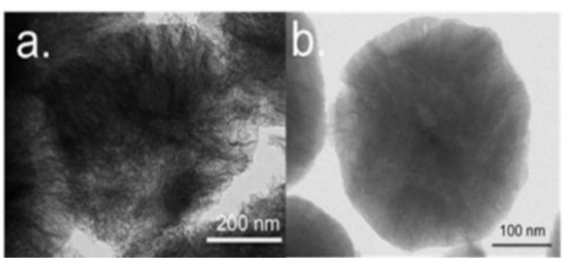
Project Duration: 7/1/2014 – 6/30/2017

Total Project Value: $249,291

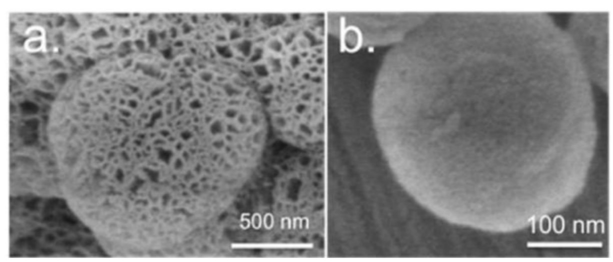
Technology Area: University Training and Research

NETL is partnering with Delaware State University to develop a better solid sorbent for carbon capture from flue gas. A nanosheets-made silica nanosphere (NSN) sorbent and an improved amine-containing NSN (PolyNSN) sorbent with amine functionality will be formulated. The research aims to demonstrate a nanosheets-made silica nanosphere (NSN) platform as a solid sorbent with spatial control of CO_2 capture amine functionality and high amine loading of at least 7 mmol N/g sorbent, with hybrid absorption-adsorption capacity of at least 5 mmol CO_2 per gram of NSN sorbent. This will be accomplished by performing parametric and long-duration tests to demonstrate that the technology meets the performance target of achieving of CO_2 capture at greater than 90% from simulated flue gas with 15% CO_2; engineering a gate-keeping polymeric layer of NSN surface (PolyNSN) designed to increase selectivity of CO_2 capture by excluding N_2 in the capture process; and finally performing parametric and long-duration tests to demonstrate proof-of-concept of nitrogen exclusion in selective CO_2 capture in PolyNSN.

The research could lead to the development of efficient CO_2 capture technologies. The materials developed will remove CO_2 from air in existing fossil-burning plants. It will also aid in the development of inexpensive CO_2 adsorbents that could solve issues associated with the operation of alkaline fuel cells.



TEM images of NSN-1 (a) and NSN-3 (b) showing the nanosheet-structure of the two novel materials.



SEM images of materials NSN-1 and NSN-3.

Novel Low Cost Environmentally Friendly Synthetic Approaches toward Core Shell Structured Micro-Particles for Fossil Energy Applications

Performer: Howard University

Collaborator(s): The Ohio State University

Award Number: FE0011515

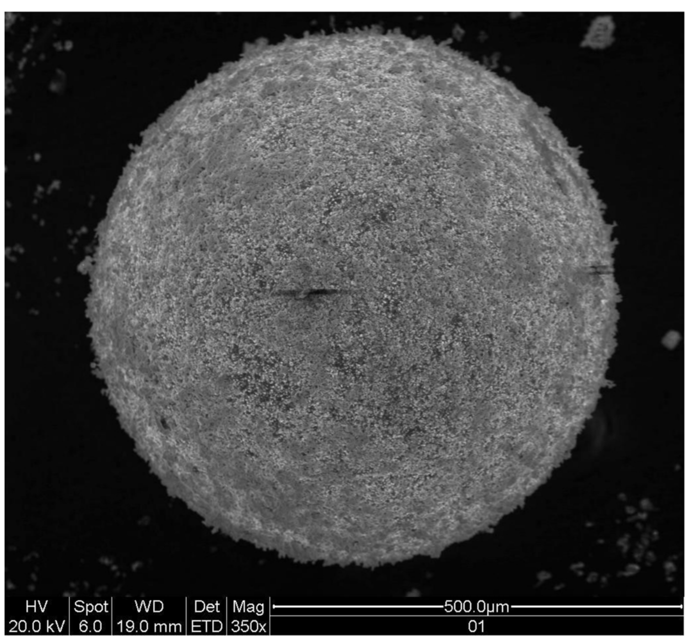
Project Duration: 7/1/2013 – 6/30/2015

Total Project Value: $199,892

Technology Area: University Training and Research

NETL is partnering with Howard University for this project. The Department of Chemistry at Howard University (HU) and the subcontractor, Ohio State University (OSU) Department of Chemical Engineering, will collaborate to investigate two novel synthetic methods toward the preparation of core-shell structured particles for applications in chemical looping combustion/gasification and postcombustion CO_2 capture. The proposed methods of preparation, metal organic chemical vapor deposition (MOCVD) and ionic diffusion are both low cost and environmentally friendly when compared to other fabrication methods. HU will synthesize and characterize CVD precursors and utilize them in the CVD growth of iron oxide. The grown core-shell structured particles will be fully characterized utilizing scanning electron microscopy-energy dispersive x-ray, atomic force microscopy (ATM), and transmission electron microscopy. OSU will investigate the ionic diffusion synthetic approach and evaluate the catalytic activity of the synthesized particles.

Completion of the proposed work will introduce a novel, low-cost and environmentally-friendly synthetic strategy for the preparation of core-shell particles. This will benefit not only the chemical looping combustion/gasification and postcombustion CO_2 capture as demonstrated in this study, but also many other related fossil energy conversion processes.



SEM analysis on 40 percent iron oxide loading particle.

Influence of Processing on Microstructure and Properties of Iron Aluminides and Coatings

Performer: Idaho National Laboratory

Award Number: FWP-1168-100159

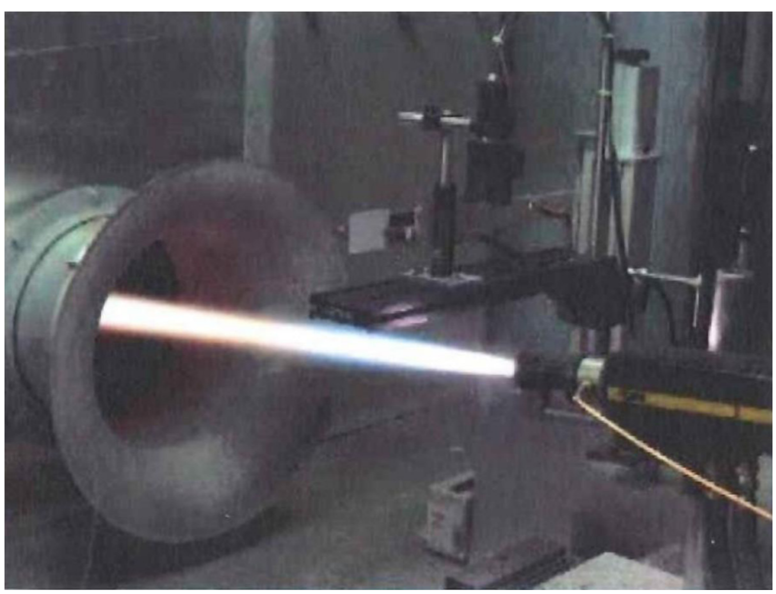
Project Duration: 10/1/2009 – 9/30/2014

Total Project Value: $441,000

Technology Area: Plant Optimization Technologies

NETL partnered with the Idaho National Laboratory on this project. The Idaho National Laboratory has a long history in the area of thermal spray coatings; research has focused on assessing the impact of various thermal spray parameters on coating characteristics (such as coating porosity, coating microstructure, and residual stress in the coating), developing coating compositions that resist environmental degradation and thermal spray diagnostics. Advanced coatings impart environmental degradation resistance to high-temperature structural alloys that may not otherwise have the corrosion resistance necessary for use in modern, high-efficiency, fossil-energy power plants. This project determined the influence of thermal spray processing parameters on the microstructure, stress state, and performance of advanced coatings for high temperature corrosion and oxidation resistance in fossil energy applications. Coating performance tests included measures of coating adhesion and durability and corrosion/oxidation resistance under constant and cyclic temperature conditions.

The project's goal was to increase the efficiency of power production from fossil fuels by enabling plant operation at higher temperatures. The optimized thermal spray methods developed by this project may extend the use of thermal and environmental barrier coatings in fossil energy power production. These coatings will permit the cost-effective operation of power plants at the elevated temperatures and pressures required to meet DOE's efficiency and emissions targets.



The high-velocity oxy-fuel thermal spray device at work.

Novel Functionally-Graded Thermal Barrier Coatings in Coal-Fired Power Plant Turbines

Performer: Indiana University

Award Number: FE0008868

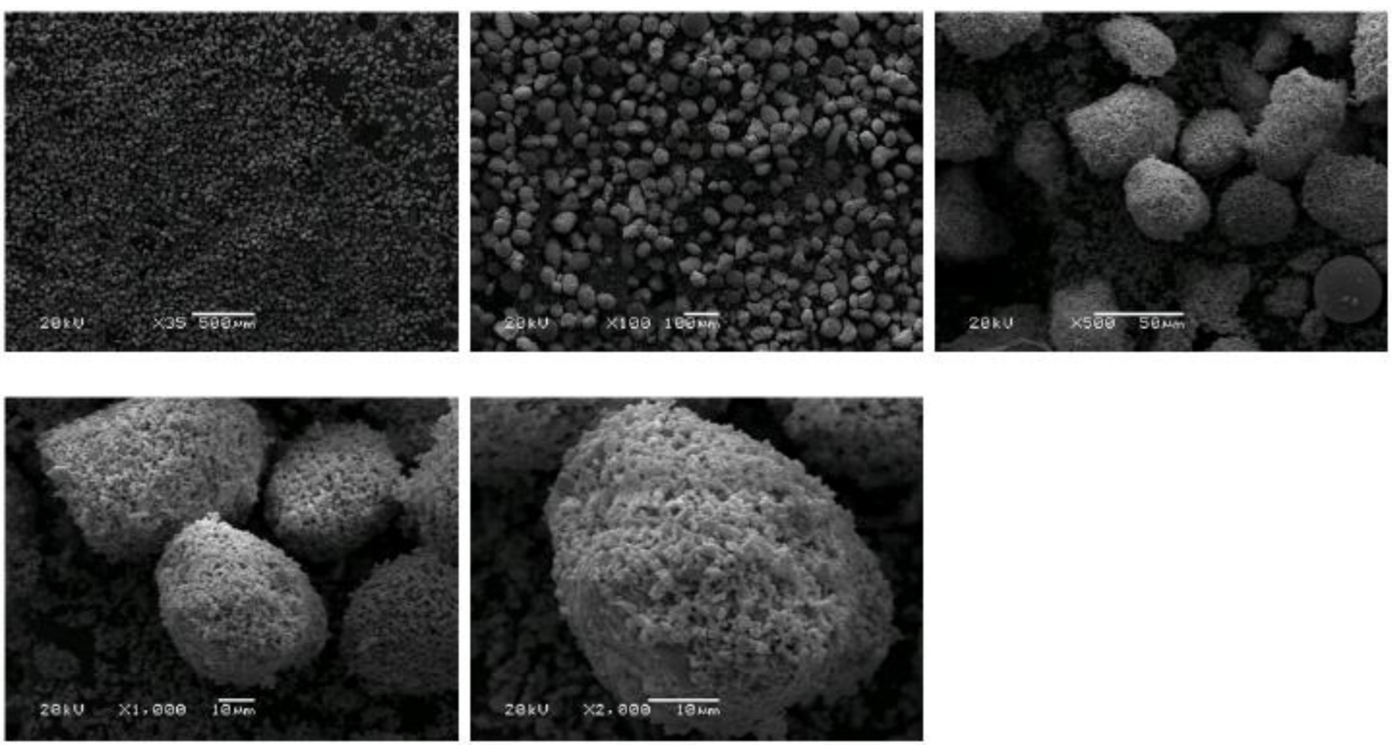
Project Duration: 9/1/2012 – 8/31/2015

Total Project Value: $293,519

Technology Area: University Training and Research

NETL is partnering with Indiana University to investigate in detail a novel double-layer functionally graded coating material, pyrochlore oxide for thermal barrier coatings (TBC). The overall objective of this research is to develop a manufacturing process to produce the novel low thermal conductivity and high thermal stability pyrochlore oxide-based double-layer coatings with improved high-temperature corrosion resistance. Novel double-layer functionally graded TBCs will be fabricated using high velocity oxy-fuel thermal spray and/or air plasma spraying technology. The TBC materials will be characterized, their corrosion resistances at elevated temperature and corrosive environments will be evaluated, and their performance under corrosive environments at high temperatures will be measured. Additionally, parameters that affect residual stresses in TBC laminates, such as composition and thickness of layers will be identified. Laminated materials with the desired bulk residual stresses will be designed and their failure mechanisms and mechanical performances will be studied. Finally, a computational model to predict residual stress in the TBCs will be developed.

Compared with the current standard TBC, partially yttria-stabilized zirconia (PYSZ), pyrochlore oxides $A_2^{3}+B_2^{4}+O_7$ (e.g., $La_2Zr_2O_7$, $Nd_2Zr_2O_7$, $Sm_2Zr_2O_7$, $Gd_2Zr_2O_7$) have demonstrated lower thermal conductivity and better thermal stability, which are crucial to the high-temperature applications such as in coal-fired power plant turbines.



FEM images of the 53 micron size powder at various magnifications.

Rational Design of Mixed-Metal Oxides for Chemical Looping Combustion of Coal Via Computational Experimental Studies

Performer: North Carolina State University

Award Number: FE0011247

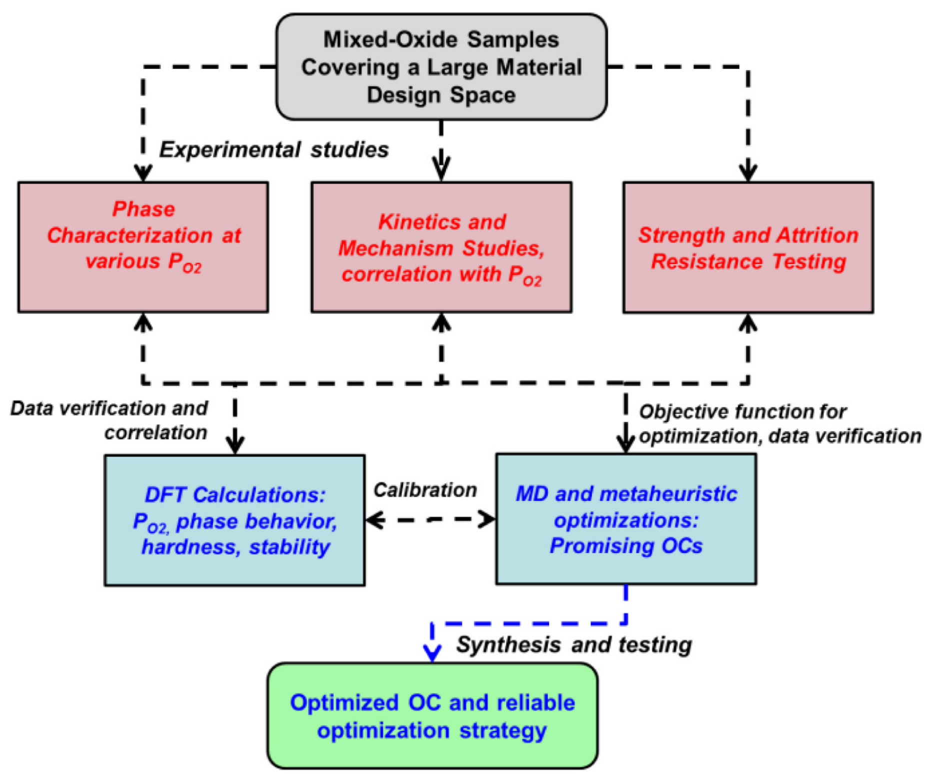
Project Duration: 9/15/2013 – 9/14/2016

Total Project Value: $363,404

Technology Area: University Training and Research

NETL is partnering with North Carolina State University to perform experimental and simulation studies to develop a systematic approach to quantify the relationships among the compositional, structural, and reactive properties of the oxygen carriers (OCs) that will lead to a systematic approach and quantitative criteria for oxygen carrier development. The studies will include multi-scale modeling, metaheuristic optimization, and experiments to design optimized OCs for coal chemical-looping combustion. A combination of experimental techniques, including x- ray/neutron diffraction, x-ray photoelectron spectroscopy, in-situ diffuse reflectance infrared Fourier transform spectroscopy, temperature programmed reduction/oxidation/desorption, and gravimetric titration techniques will be utilized to comprehensively study the bulk and surface redox reaction mechanisms and phase behaviors of the OCs. Ab-initio and molecular dynamics simulations will be used to predict material properties, and metaheuristic optimization algorithms will be used to identify promising OC candidates. An effective metaheuristic optimization algorithm will be developed through experimental validation and calibration.

This project will result in published methods and development of computer tools to create optimized OC materials with superior properties; accurate and effective strategies for computer assisted OC material design; and synthesis of nine or more mixed oxides with good oxygen uncoupling properties and desired structures such as bixbyite, spinel, and perovskite. Researchers will be able to accurately predict the relationship between mixed-oxide compositions and their phase properties for OC optimization.



Schematic of the proposed scientific approach.

Reduced Cost Bond Layers for Multi-Layer Thermal/Bespoke Materials Surfaces

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA105

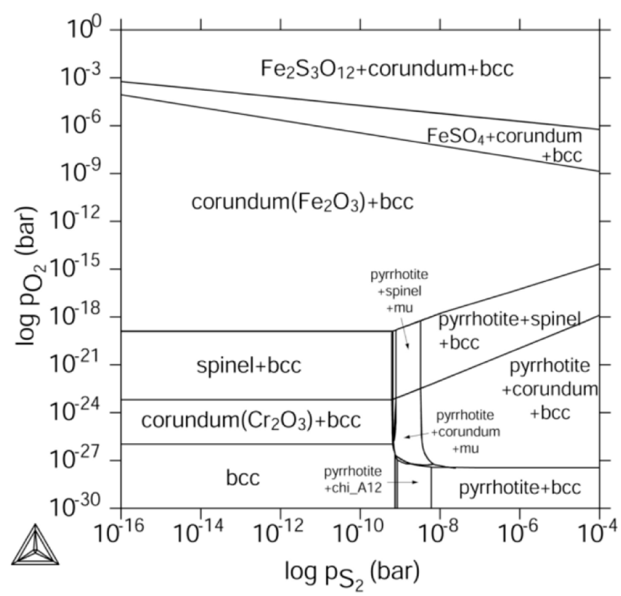
Project Duration: 10/1/2009 – 9/30/2014

Total Project Value: $1,087,500

Technology Area: Plant Optimization Technologies

NETL partnered with Oak Ridge National Laboratory to develop coatings capable of withstanding the extreme conditions in the furnace zone of coal-fired boilers, where large areas of waterwall tubes are subjected to staged combustion conditions for nitrogen oxide (NO_x) reduction. In this project, ORNL researchers developed a family of material coatings to address coal-fired waterwall tube fireside protection, determined how surfaces and interfaces affect selected properties, and investigated how the desired combination of properties can be incorporated into a coating and a process for its deposition.

The goal was the development of bespoke (tailored) materials surfaces that have a combination of good adherence, high resistance to fireside corrosion, and minimum effect on thermal conductivity, and can be tailored for easy application to the waterwall tubes of coal-fired boilers to provide effective protection from corrosion and thermal fatigue. This project identified coating materials and application techniques that have the potential to cost-effectively protect coal-fired boiler waterwall tubes in a high-temperature, high-pressure and corrosive operating environment.



Calculated stability diagram for a low chrome-iron alloy (Fe-2.25Cr-1Mo) at 800 °C using Thermo-Calc™ software equilibrated under the indicated sulfur and oxygen partial pressures. The diagram shows the different metals, metal oxides, and metal oxy-sulfide compounds that will exist at 800 °C.

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

Performer: Prairie View A&M University

Award Number: FE0023040

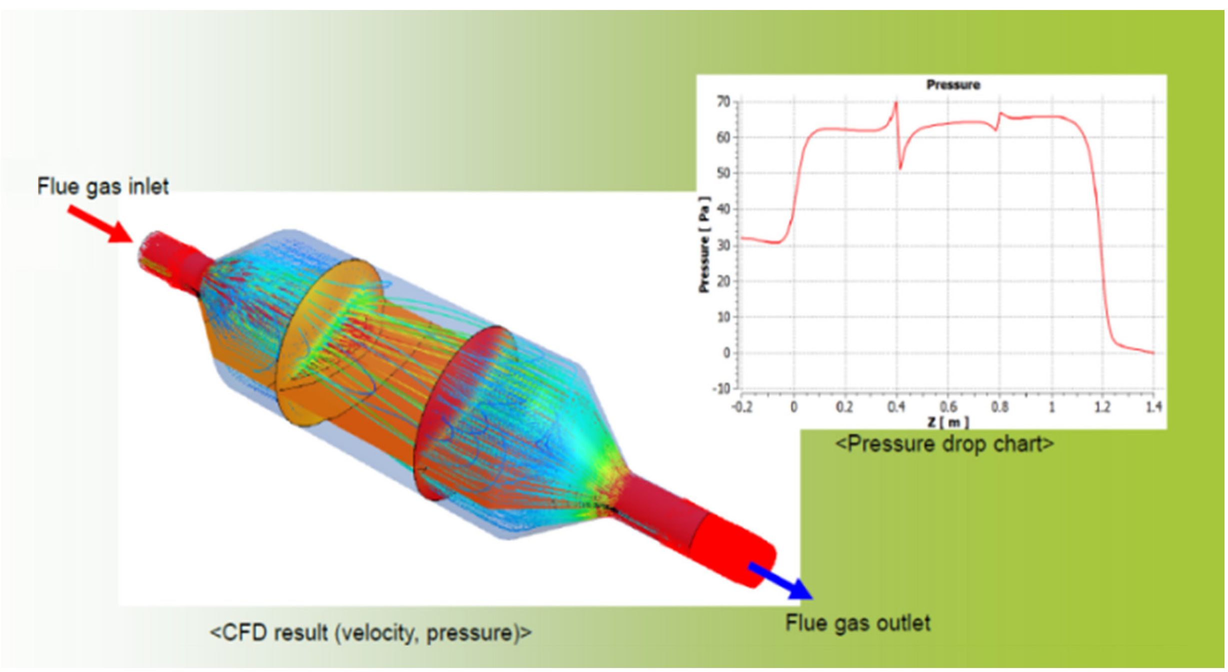
Project Duration: 10/1/2014 – 9/30/2017

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 on the synthesis of titanium dioxide (TiO_2) nanotubes and adsorption characteristics of polyethylenimine (PEI) and also 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 work 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 and low cost method to capture CO_2 from effluents of advanced fossil energy systems.



CFD Modeling: Porous Media.

Courtesy of Prairie View A&M University.

HVOF Thermal Spray TiC/TiB_2 Coatings of AUSC Boiler/Turbine Components for Enhanced Corrosion Protection

Performer: Southern Illinois University

Award Number: FE0008864

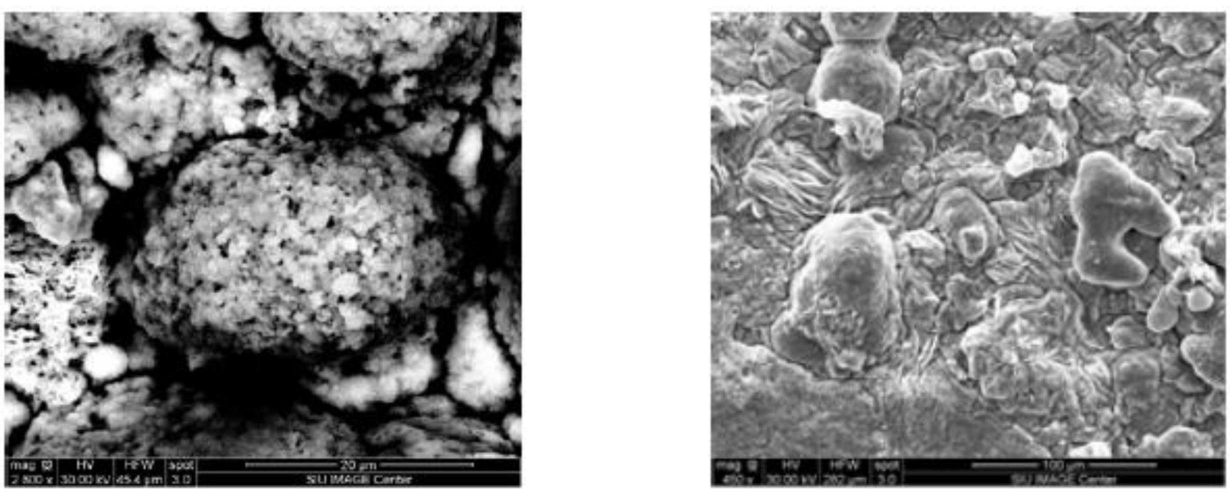
Project Duration: 9/1/2012 – 8/31/2015

Total Project Value: $442,212

Technology Area: University Training and Research

NETL is partnering with Southern Illinois University to develop TiC- and TiB_2-based coatings applied via high velocity oxygen fuel (HVOF) thermal spray method onto various substrates used in boilers and turbines operating under ultrasupercritical steam conditions. The specific objectives of the project are (1) synthesis of nanoparticles of TiC by a patented process, (2) extension of the process to synthesize nano-sized TiB_2 powder, (3) optimization of HVOF spray coating of the TiC and TiB_2 on select ferritic, austenitic, and nickel alloy samples generally used for water-wall tubing, high temperature boiler sections, turbine blades, and USC tubing applications, (4) laboratory evaluation of the corrosion resistance of the coatings employing simulated flue gas and simulated ash, (5) selection of optimal alloy protection system in different temperature/chemical regimes, and (6) field evaluation of fabricated probes of select coating in actual boiler/turbine environment.

A demonstration of the TiC- and TiB_2-based coatings applied via HVOF thermal spray method will enable new technology innovation and finer quantitative control of coating performance to meet stringent requirements for use in advanced ultrasupercritical boiler, steam turbine, and gas turbine operational environments.



SEM image of surfaces after exposure to simulated ash environment after 800 hours (left – uncoated, right -coated).

An Integrated Study of a Novel Thermal Barrier Coating for Niobium-Based High Temperature Alloy

Performer: Southern University and A&M College

Award Number: FE0007220

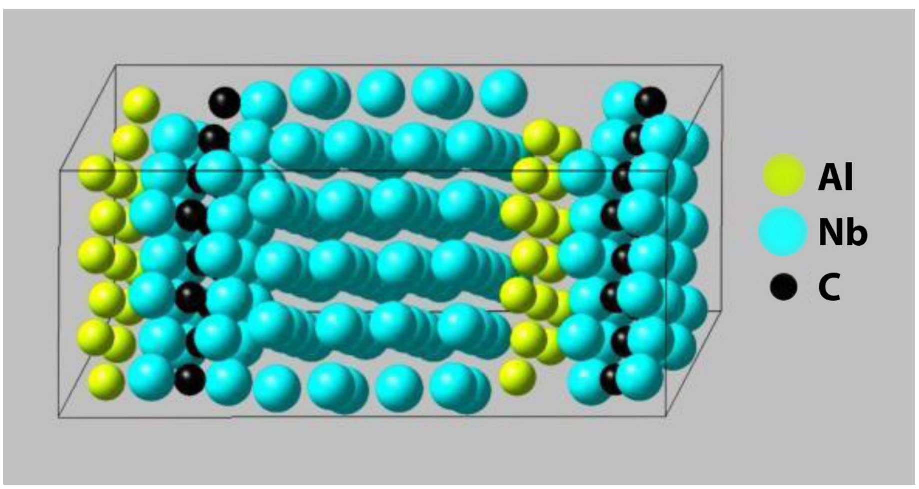
Project Duration: 10/1/2011 – 1/31/2015

Total Project Value: $200,000

Technology Area: University Training and Research

NETL partnered with South University and A&M College to integrate high performance computer (HPC) simulation and experimental validation in material sciences to study the elastic constants, interface bonding, high-temperature microstructures, melting points, diffusion coefficients, and oxidation resistance of the proposed bond coat and top coat of Nb-based alloys. Specific objectives for the project were: (1) perform interface energy HPC simulation on the bond coat/Nb-based alloy and top coat/bond coat interface models to screen potential bond coat candidates; (2) study the high-temperature properties and oxidation resistance capabilities of the bond coat/top coat Nb-based alloys through molecular dynamics simulation; and (3) perform experiments to determine the oxidation resistance of the most promising systems from the simulation.

The result of this project will enhance U.S. energy security by integrating HPC simulation and experimental validation in material sciences that will make it possible to maintain a cost-competitive, environmentally acceptable, coal-based power generation option. Project results will enhance the ability of domestic boiler manufacturers to successfully build high-efficiency boilers for both domestic and international coal-fired power plant operators.



An interface model of Nb2AlC(001)/Nb(110) interface.

Fabrication and Processing of Next Generation Oxygen Carrier Materials for Chemical Looping Combustion

Performer: University of Toledo

Award Number: FE0008774

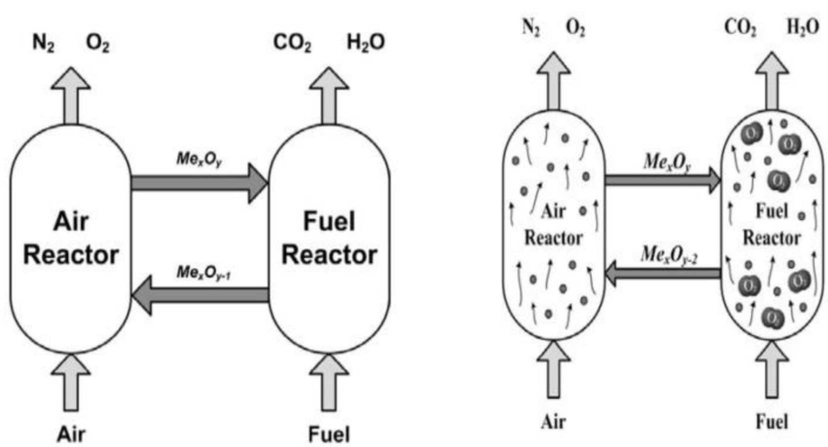
Project Duration: 9/4/2012 – 9/3/2016

Total Project Value: $470,674

Technology Area: University Training and Research

NETL is partnering with University of Toledo to combine synthesis and processing protocols to produce and characterize laboratory-scale quantities of new oxygen carrier materials. The team will perform thermogravimetric and differential thermal analysis (TG-DTA), abrasion and crush strength tests, and other analytical tests to determine the physical, structural, and chemical characteristics of these materials. Specific objectives in support of the project goal are (1) to produce laboratory-scale quantities of new oxygen carrier materials; (2) to process the materials into fluidizable form with proper size distribution; (3) to characterize the materials using a variety of analytical techniques to determine physical properties, chemical composition, and performance of the materials; and, (4) to determine the oxygen reactivity of the developed oxygen carriers with a solid fuel such as coal under typical oxidizing and reducing conditions for chemical looping combustion.

This project will develop and produce new perovskite-based oxygen carriers expected to have greater thermal and chemical stability over a wide range of temperatures and oxygen partial pressures and be environmentally safer than current materials. These new oxygen carriers may contribute to the advance of chemical looping combustion as an efficient and economical approach to fossil fuel-based combustion with carbon capture for better use of domestic energy resources with less negative impact on the environment.



Schematic description of CLC (left) and chemical looping with oxygen uncoupling (CLOU) (right) processes. In the CLC process, the metal oxide reacts directly with the fuel in the fuel reactor. In the CLOU process, the metal oxide releases the oxygen in the fuel reactor, and gaseous oxygen then reacts with the fuel.

Multi-Scale Computational Design and Synthesis of Protective Smart Coatings for Refractory Metal Alloys

Performer: University of Wisconsin

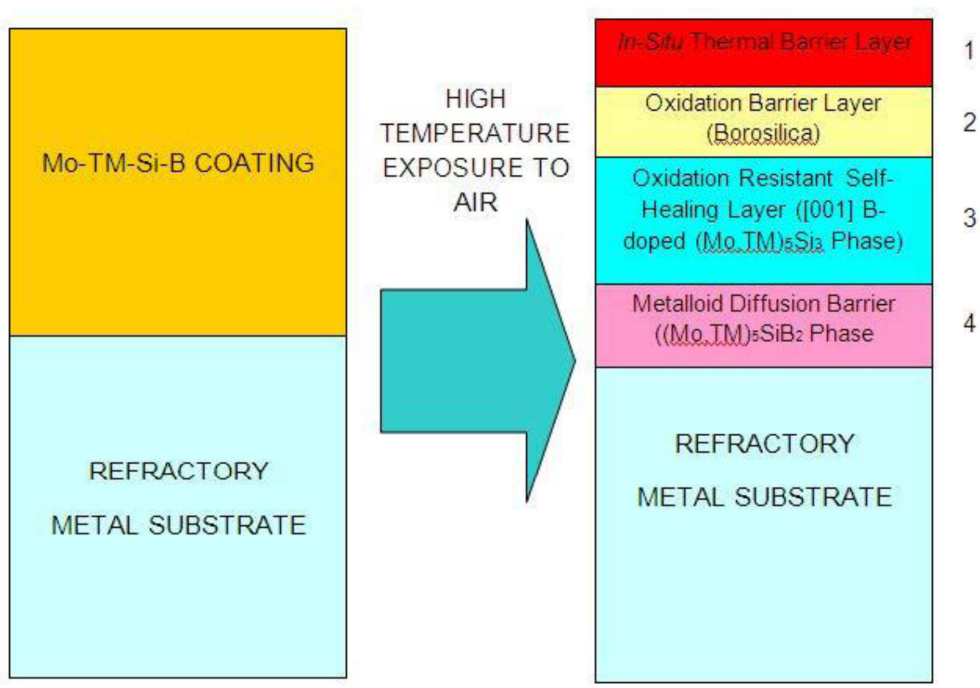
Award Number: FE0007377

Project Duration: 9/1/2011 – 8/31/2014

Total Project Value: $300,000

Technology Area: University Training and Research

NETL partnered with the University of Wisconsin to enable the full integration of a new high-temperature protective coating technology into advanced combustion systems for fossil-fuel energy generation that provides both environmental and thermal protection and a 200 to 400 °C increase in material operating temperature beyond that of current nickel-based superalloys. The enabling technology underlying this advance is based on the computational design of a novel, multifunctional integrated coating strategy that provides both environmental and thermal protection to advanced combustion systems. These improvements, when implemented, should enable power plants to deliver an increase in power efficiency by operating at higher temperatures and pressures.



Design of the Mo-TM-Si-B smart coatings based upon multi-layer structures that develop four integrated functionalities after air exposure at high temperatures.

Abbreviations

°C .... degrees Celsius

°F .... degrees Fahrenheit

3-D .... three-dimensional

AFM .... atomic force microscopy

AM .... additive manufacturing

ANL .... Argonne National Laboratory

APS .... air plasma sprayed

ASME .... American Society of Mechanical Engineers

AUSC /A-USC .... advanced ultrasupercritical

BCC .... body centered cubic

CALPHAD .... calculation of phases diagram

CCSI .... Carbon Capture Simulation Initiative

CFD .... computational fluid dynamic

CLC .... chemical looping combustion

CMAS .... calcium-magnesium-alumino-silicates

CME .... chemical and molecular engineering

CNT .... carbon nanotubes

CO_2 .... carbon dioxide

CSEF .... creep strength enhanced ferritic

CSL .... coincident side lattice

CSM .... Colorado School of Mines

CVD .... chemical vapor deposition

DOE .... [U.S.] Department of Energy

EBC .... environmental barrier coating

EPA .... [U.S.] Environmental Protection Agency

FCC .... face centered cubic

FE .... [DOE Office of] Fossil Energy

FFT .... fast Fourier transform

FSW .... friction stir welding

GB .... grain boundaries

GB/IGF .... grain boundaries/intergranular films

GE .... General Electric Company

H_2 .... hydrogen

HBCU/OMI .... historically Black colleges and universities/ and other minority institutions

HEA .... high energy alloy

HIP/PMP .... hot isostatic pressure of powdered metal

HPC .... high performance computing

HPM .... high performance materials

HU .... Howard University

HVOF .... high velocity oxy-fuel

ICWE .... integrated computational weld engineering

IGCC .... integrated gasification combined cycle [power plant]

K .... kelvin

LHVOF .... liquid fueled high velocity oxy-fuel

L-PBF .... laser powder bed fusion

LOM ... laminated object manufacturing

MASHS ... mechanically activated self-propagating high-temperature synthesis

MAX ... MAX phases, or $M_{n+1}AX_n$ [M = a transition metal, A = (Al), X = (C) or (N)]

MC ... Monte Carlo

MD ... molecular dynamics

MHD ... magneto-hydrodynamic

Mo ... molybdenum

MOCVD ... metal organic chemical vapor deposition

MOFs ... metal organic framework

MPa ... megapascals

NDE ... nondestructive evaluation

NETL ... National Energy Technology Laboratory

Ni ... nickel

NOx ... nitrogen oxide

NRAP ... National Risk Assessment Partnership

NSN ... nanosheet-made silica nanoshere

O_2 ... oxygen

OC ... oxygen carriers

ODS ... oxide dispersion strengthened

OM ... omega method

OMI ... other minority institutions

ORNL ... Oak Ridge National Laboratory

OSU ... Ohio State University

PEI ... polyethylenimine

PNNL ... Pacific Northwest National Laboratory

psi ... pounds per square inch

PWHT ... post weld heat treatment

PXRD ... powder X-ray diffraction

R&D ... research and development

ReaxFF ... reactive force field

SBIR ... Small Business Innovation Research

SEM-EDX ... scanning electron microscopy/ energy dispersive x-ray

SOFC ... solid oxide fuel cell

SQS ... special quasirandom structure

TBC ... thermal barrier coating

TEM ... transmission electron microscopy

TG-DTA ... thermogravimetric and differential thermal analysis

TiO_2 ... titanium dioxide

U.S. ... United States

UCR ... University Coal Research [NETL program]

USC ... ultrasupercritical

UTR ... University Training and Research

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http://www.netl.doe.gov/research/coal/crosscutting/simulation-based-engineering

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