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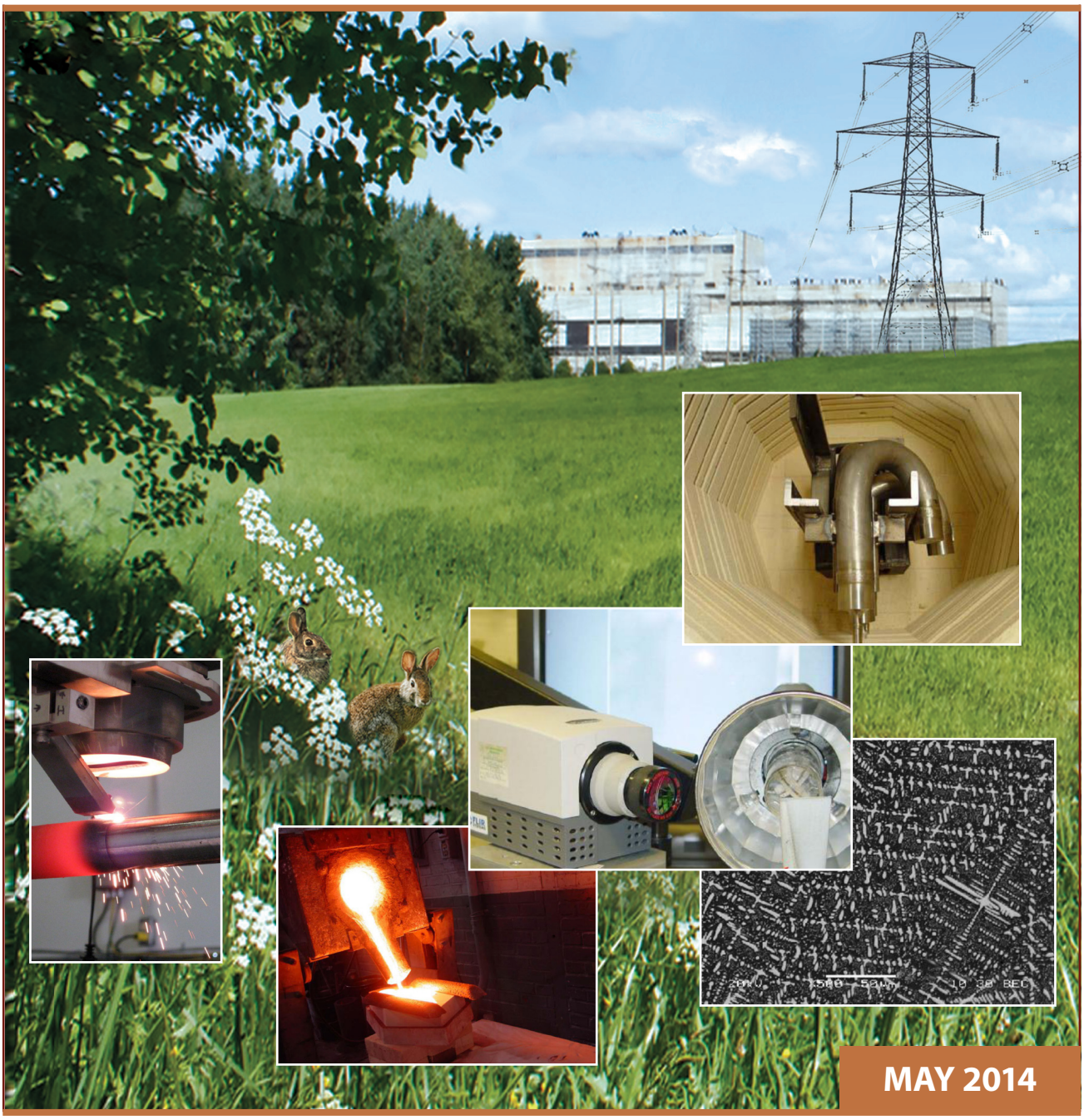
Crosscutting Research High Performance Materials Project Portfolio



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U.S. DEPARTMENT OF ENERGY

the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

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Introduction

The Crosscutting Research Program develops a range of innovative and enabling technologies that are key to improving existing power systems and essential for accelerating the development of a new generation of highly efficient environmentally benign fossil fuel based power systems.The mission space is focused on bridging the gap between fundamental and applied 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 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 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 in Advanced Energy Systems (AES) and Carbon Capture and Storage (CCS). The Crosscutting Research program comprises the following major technology thrusts:

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 in-formation networks and distributed intelligence for process control and decision making.

High Performance Materials: Materials development, under the Crosscutting Research Program, focuses on structural materials that will lower the cost and improve the performance of fossil-based power-generation systems. Computational tools to support 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 phenomenon occurring in fossil fuel conversion processes and development of multi-scale, 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 innovative 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.

Environmental Control is based on a legacy program that encompassed the development of advanced mercury and NO_X emissions control technologies, coal utilization byproduct (CUB) research, to CO_2 emissions control for existing plants and Water-Energy Interface R&D. This area made significant contributions to lowering the environmental impact of coal based power systems. Efforts are underway to analyze the future impacts of water for advanced power systems and how R&D can address these pending issues.

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

Coal Utilization Sciences: The Coal Utilization Sciences technology area research effort is being 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 serve to 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 UTR program sponsors research based educational grants to U.S. Universities and Colleges in areas that benefit the Office of Fossil Energy and the Crosscutting 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 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 enacted 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.

This project portfolio report showcases 53 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.

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.

Specific Technology Objectives:

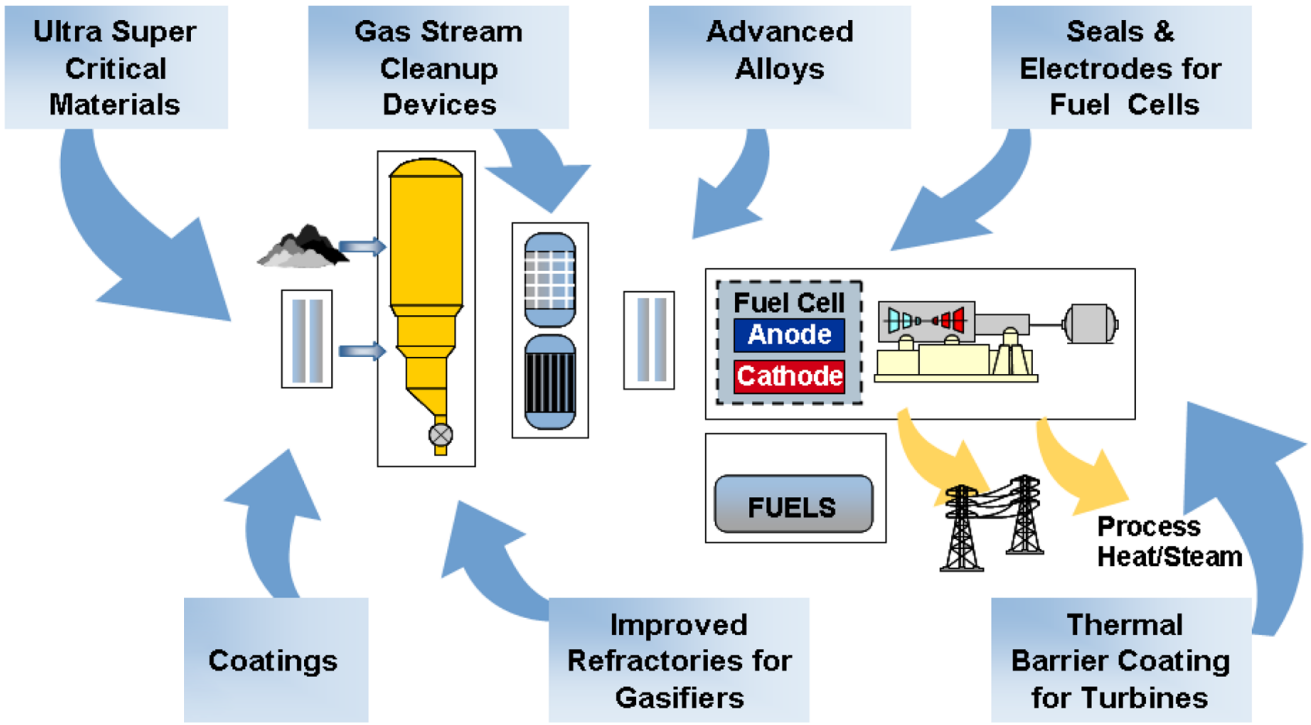
- Development of computational materials modeling to enable rapid design and simulation of new and novel alloy materials with less repetitive testing. Computational design of materials has the potential to produce major breakthroughs

- 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.

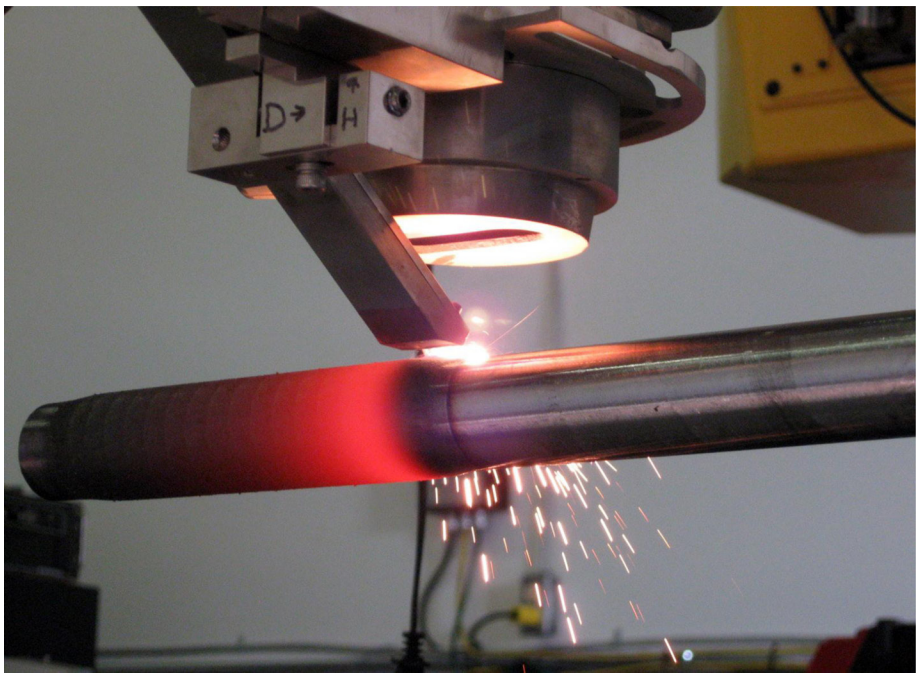


High Performance Materials research areas.

Projects by Component Technologies

Coatings/Protection Materials

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.



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Materials Research for Coal Conversion and Utilization Processes—Corrosion and Mechanical Properties of Materials in Combustion and Mixed-Gas Environments

Performer: Argonne National Laboratory (ANL)

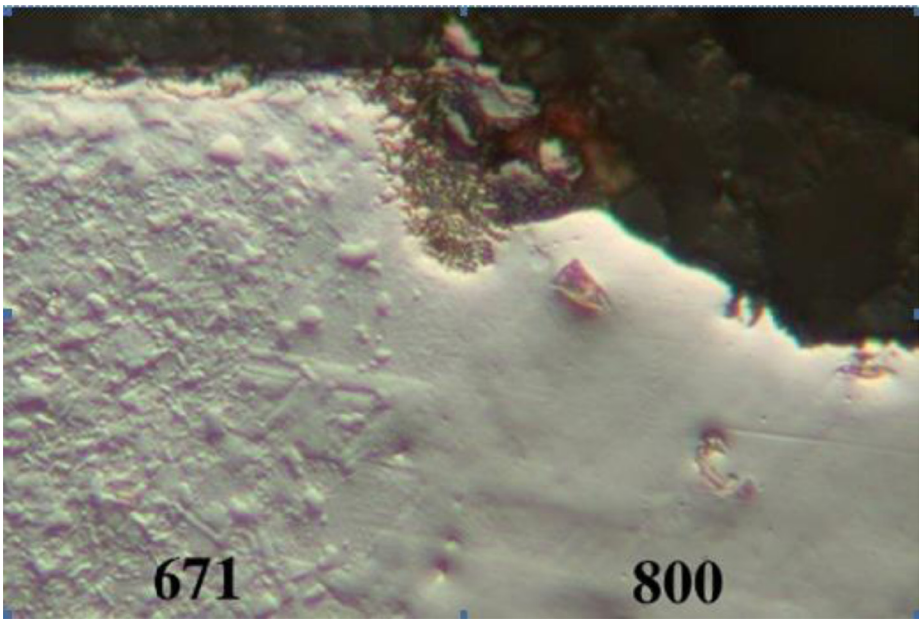
Award Number: FWP 49640

Project Duration: 10/01/2006–09/30/2015

Total Project Value: $1,225,000

Funding Source: Plant Optimization Technologies

The work being conducted under this project will provide a basic understanding of the protective scale formation mechanisms, the microstructural characteristics of scales, their sulfur and chlorine resistance, and the causes and mechanisms for scale breakdown in complex gas environments and in the presence of deposits. Experiments will establish the corrosion behavior of several materials that have been developed for advanced steam-cycle application with emphasis on the role of alloy composition in scale development and adhesion, as well as breakaway phenomena leading to scale failure. In particular, the effect of deposits of various chemistries on the corrosion performance of the alloys will be evaluated.



Photomicrograph of a welded sample of alloys 671 and 800 after 668 hours exposure in an environment containing coal-ash at 650 °C.

Environmental Barrier Coatings

Performer: Auburn University

Award Number: FE0011245

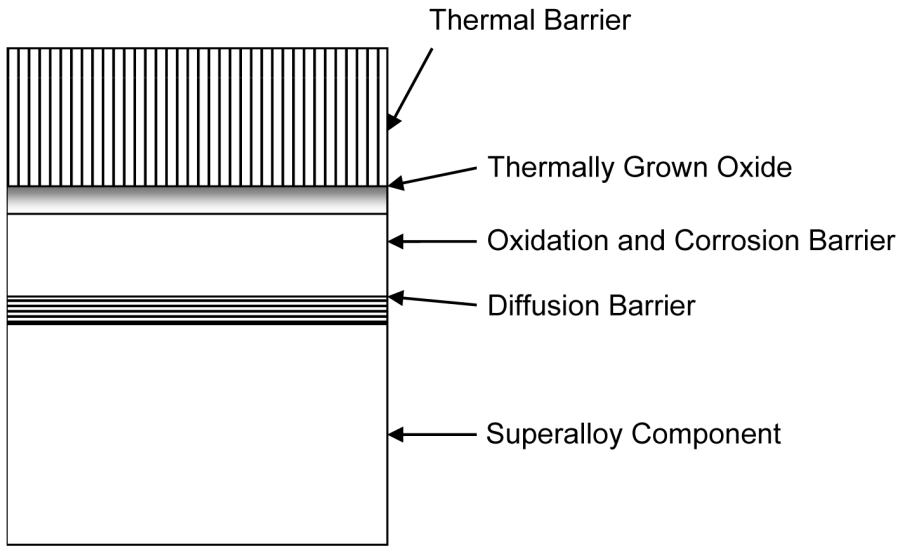
Project Duration: 7/17/2013–7/16/2016

Total Project Value: $362,310

Funding Source: 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

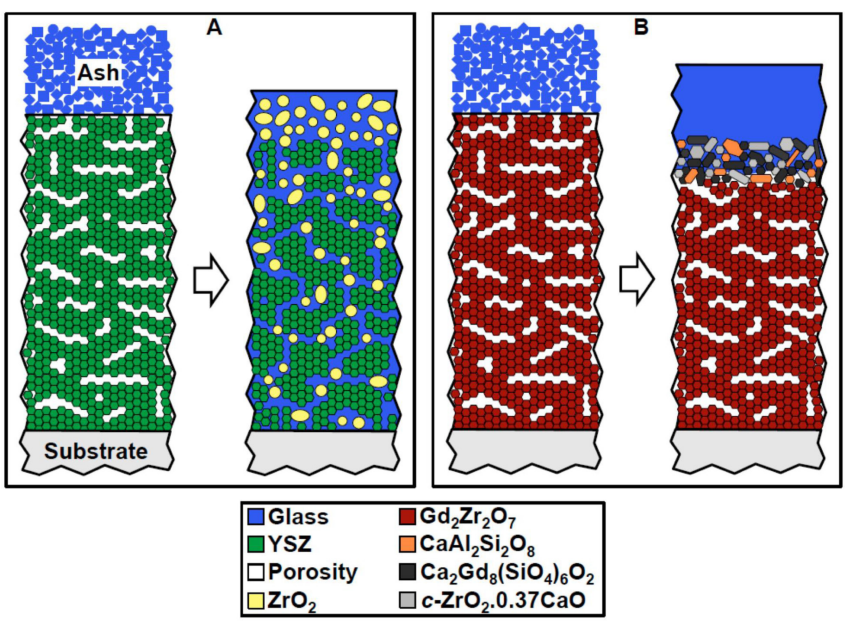
Project Duration: 9/1/2012 – 8/31/2015

Total Project Value: $324,400

Funding Source: 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.

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

Performer: Idaho National Laboratory

Award Number: FWP-1168-100159

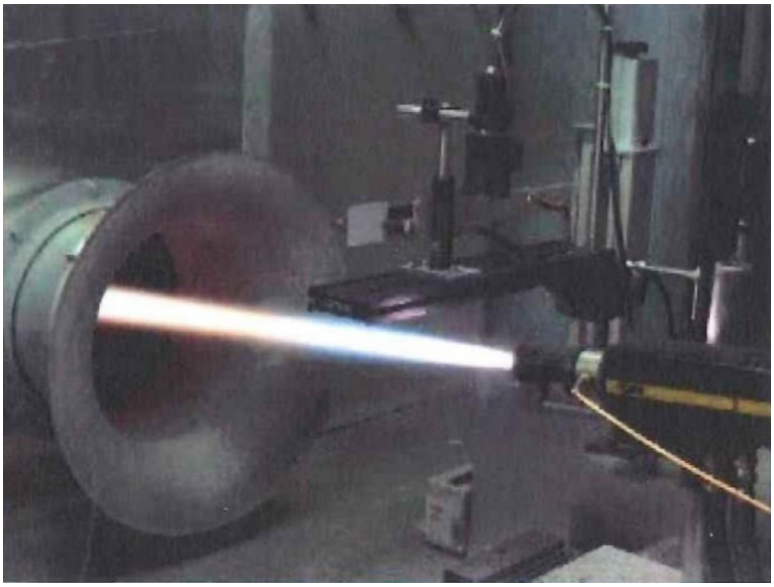
Project Duration: 10/01/2009–09/30/2014

Total Project Value: $441,000

Funding Source: Plant Optimization Technologies

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 will determine 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 will include measures of coating adhesion and durability and corrosion/oxidation resistance under constant and cyclic temperature conditions.

The project's goal is to increase the efficiency of power production from fossil fuels by enabling plant operation at higher temperatures. An effective test suite and optimized thermal spray methods and materials will contribute to 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

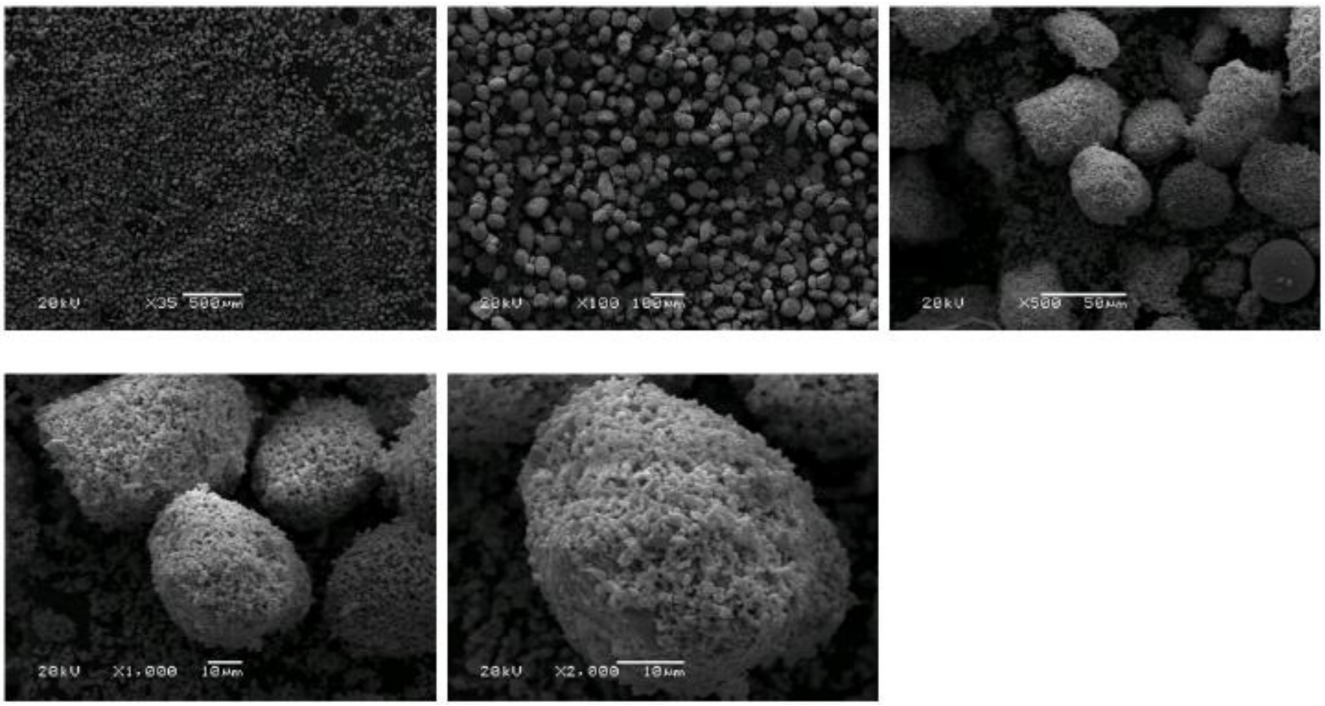
Project Duration: 9/1/2012–8/31/2015

Total Project Value: $293,519

Funding Source: 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 53 micron-sized powder at various magnification.

Bespoke Materials Surfaces

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA105

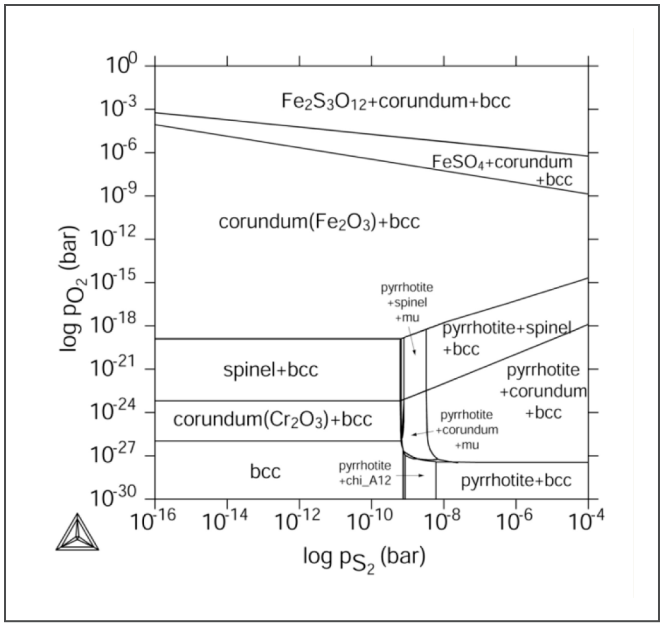
Project Duration: 10/01/2009–09/30/2014

Total Project Value: $1,087,500

Funding Source: Plant Optimization Technologies

NETL is partnering 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 will develop a family of material coatings to address coal-fired waterwall tube fireside protection, determine how surfaces and interfaces affect selected properties, and investigate how the desired combination of properties can be incorporated into a coating and a process for its deposition.

The goal of this project is to develop 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 will identify 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.

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

Performer: Southern Illinois University

Award Number: FE0008864

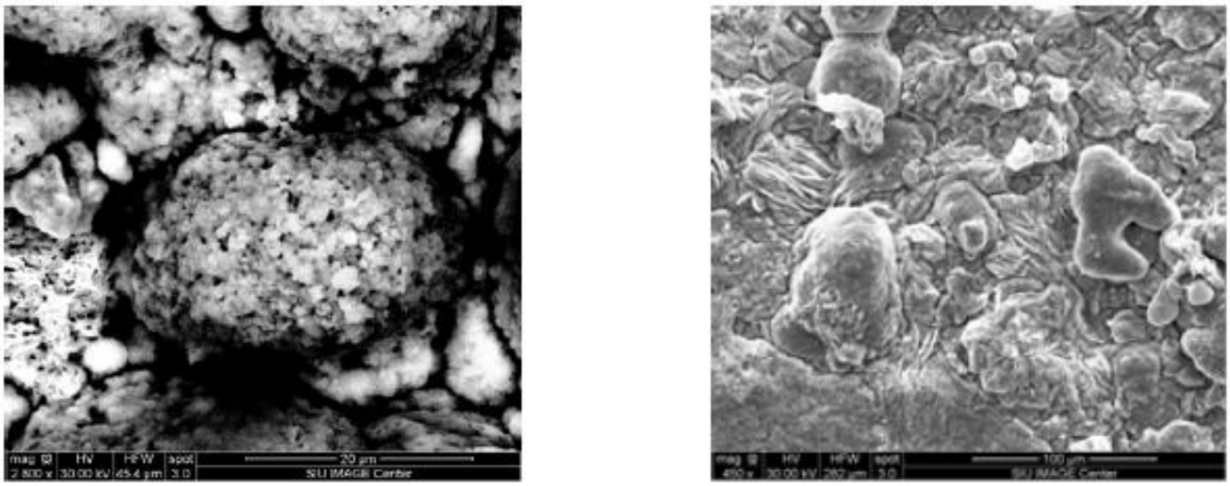
Project Duration: 9/1/2012 – 8/31/2015

Total Project Value: $442,212

Funding Source: University Training and Research

NETL is partnering with Southern Illinois University to develop titanium carbide (TiC)- and titanium diboride (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

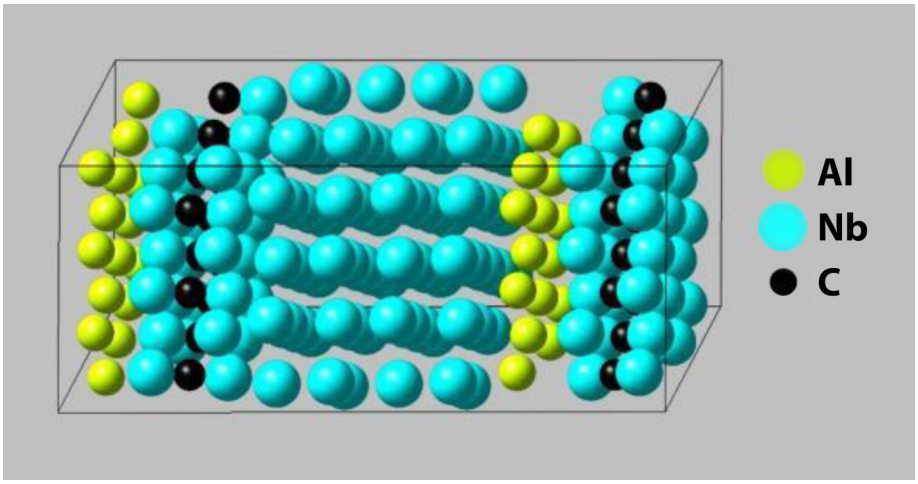
Award Number: FE0007220

Project Duration: 10/1/2011 – 5/31/2014

Total Project Value: $200,000

Funding Source: University Training and Research

NETL is partnering 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 niobium (Nb)-based alloys. Specific objectives for the project are: (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. 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 success 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 $Nb_2AlC(001)/Nb(110)$ interface.

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

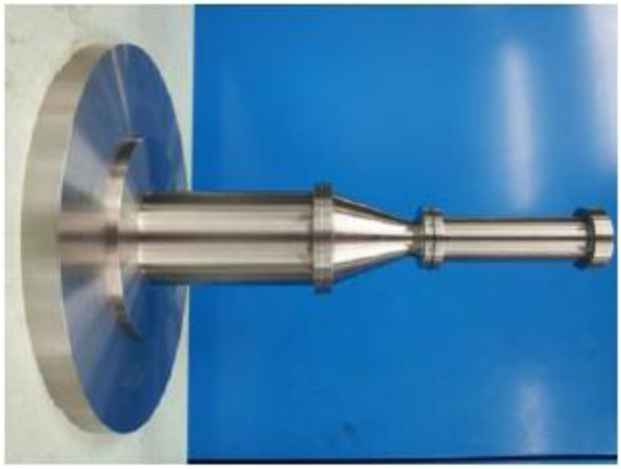
Project Duration: 7/1/2013 – 6/30/2015

Total Project Value: $200,000

Funding Source: University Training and Research

NETL is partnering with University of Texas at El 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.



An actual HVOF gun after manufacturing process (without the injector and cooling jacket sections).

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

Performer: University of Wisconsin

Award Number: FE0007377

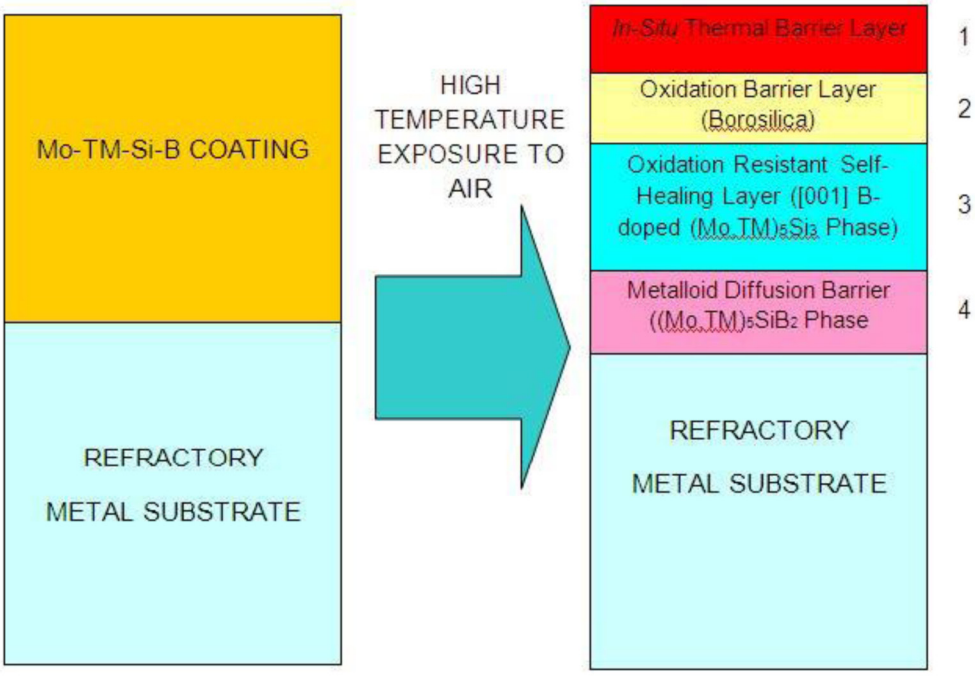
Project Duration: 9/1/2011–8/31/2014

Total Project Value: $300,000

Funding Source: University Training and Research

NETL is partnering 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 Ni-based superalloys. The enabling technology underlying this advance is based on the computational design of a novel, multifunctional integrated coating strategy that will provide 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.

New Alloys

The objective of the New Alloys research area is to increase the temperature capability of alloys for use in specific components required for advanced power plants by understanding the relationships among composition, microstructure, and properties.

Performer	Project Title	Page
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Computational and Experimental Development of Novel High-Temperature Alloys

Performer: Ames National Laboratory

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

Project Duration: 10/01/2009–09/30/2014

Total Project Value: $575,000

Funding Source: Plant Optimization Technologies

NETL is partnering with Ames 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.

The micrograph of a selected alloy shows the skeleton-like framework required for good performance in these applications.

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

Performer: Dartmouth College

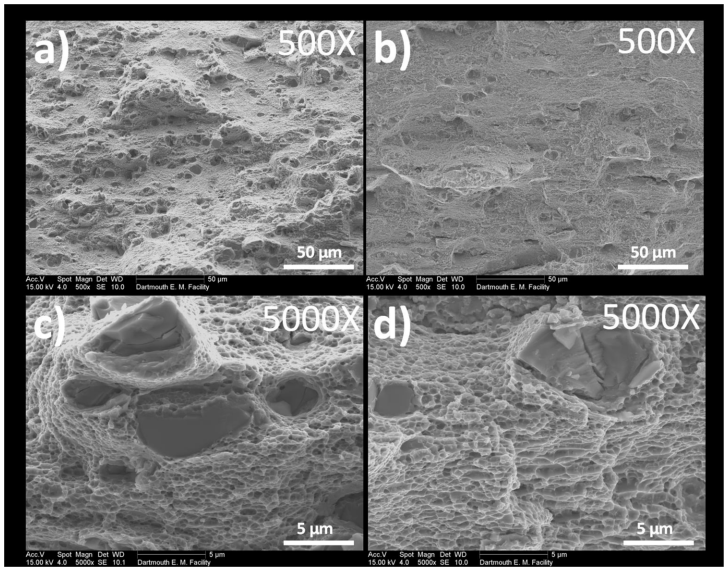
Award Number: FE0008857

Project Duration: 9/1/2012–8/31/2015

Total Project Value: $402,467

Funding Source: 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 -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.



SE image from fracture surface of sample after cold rolling and annealing at 800 ˚C for 2.4 h (a, c) after thermo-mechanical treatment method #1, and (b, d) after thermo-mechanical treatment method #2.

Oxy-Combustion Environment Characterization: Fireside Corrosion

Performer: National Energy Technology Laboratory Office of Research and Development

Award Number: FWP-2012.03.01

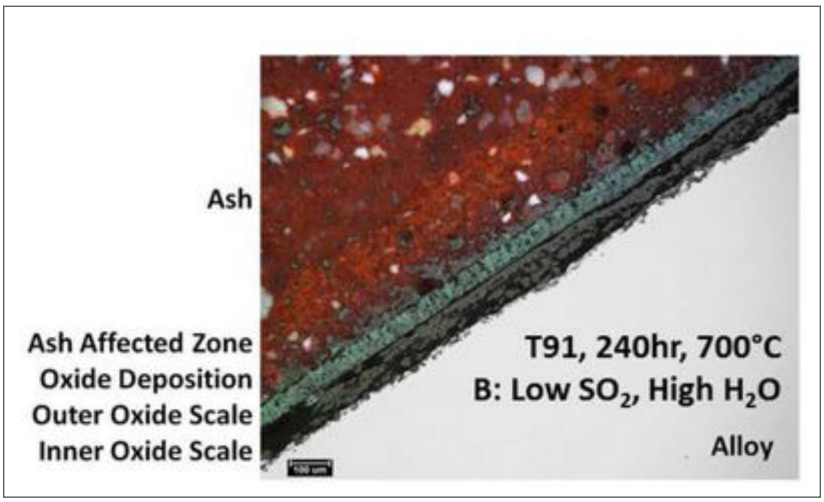
Project Duration: 10/1/2013–09/30/2014

Total Project Value: $388,000

Funding Source: Plant Optimization Technologies

This project focuses on evaluation of fireside corrosion and steam-side oxidation in oxy-combustion systems. Identification of alloys that can withstand the harsh physical and chemical conditions associated with oxy-combustion environments will lead to decreases in operating costs. Specifically, experiments will be conducted to elicit information as to the best oxy-fuel combustion designs, such as flue gas recycle sources and the use of staged combustion burners.

Several oxy-fuel combustion design issues impact fireside corrosion. Low temperature flue gas resulting from oxy-firing is divided and a portion recycled back into the boiler and a remainder processed for carbon capture. The efficiency of flue gas recycle paths is inversely proportional to expected corrosion within the boiler. Quantifying these corrosion implications is important to maintaining the efficiency of the boiler, and thus keeping the cost of electricity low. Implementation of oxy-fuel combustion concurrent with an A-USC steam cycle will require the examination of the fireside corrosion at higher superheater and reheater temperatures than in conventional boilers and of candidate A-USC boiler alloys such as the newly code-cased alloy 740. This task will provide the NETL program with published fireside corrosion rates and behavior for USC and A-USC alloys in conventional and oxy-fuel combustion environments. It will also provide data on the effect of oxy-fuel flue gas recycle on the fireside corrosion behavior of boiler tubing.



Commercial boiler tube alloy T91 after exposure at 700 °C for 240 hours in Oxy, FGD with 20 percent H_2O.

Oxy-Combustion Environment Characterization: Steamside Oxidation

Performer: National Energy Technology Laboratory Office of Research and Development

Award Number: FWP-2012.03.01

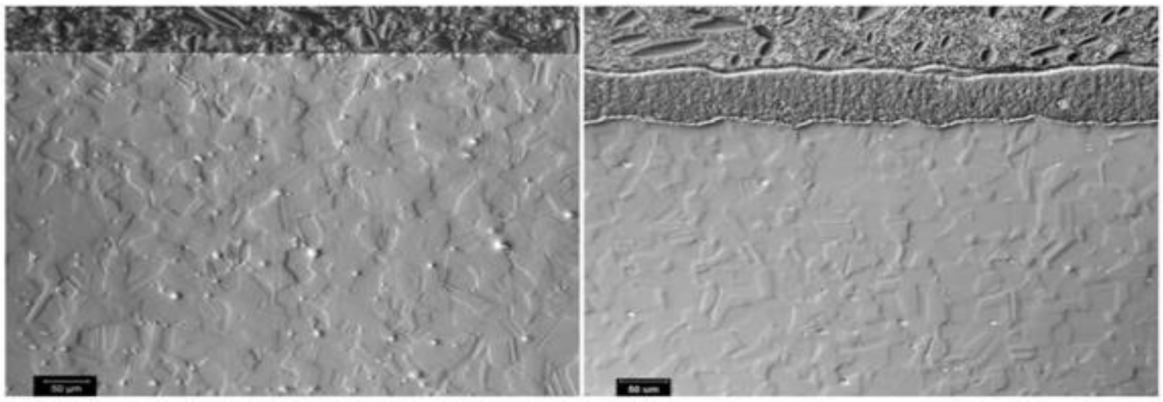
Project Duration: 10/1/2013–09/30/2014

Total Project Value: $238,000

Funding Source: Plant Optimization Technologies

This project focuses on evaluation of fireside corrosion and steam-side oxidation in oxy-combustion systems. Identification of alloys that can withstand the harsh physical and chemical conditions associated with oxy-combustion environments will lead to decreases in operating costs. Specifically, experiments will be conducted to elicit information as to the best oxy-fuel combustion designs, such as flue gas recycle sources and the use of staged combustion burners.

There is a wealth of steam oxidation data at atmospheric pressure, including data on A-USC candidate alloys. However, there is much less data available above atmospheric pressure. Steam boiler experience provides information on existing boiler alloys, but with hard-to-characterize histories. Laboratory data at pressure is limited and is either at subcritical conditions or at lower temperatures than A-USC conditions. The NETL A-USC steam autoclave provides a unique capability to examine long-term steam oxidation as a function of pressure, including A-USC conditions. There are open questions as to what happens to hydrogen during steam oxidation. As hydrogen can influence mechanical properties in alloys, knowing the injection rate into the alloy is an important consideration for the development of models to address mechanical properties in conjunction with the environmentally induced degradation. This research activity will provide the NETL program with documentation showing steam oxidation degradation rates for A-USC alloys at temperatures up to 760 ˚C, and pressures up to 34.5 megapascals (MPa).



(a) (b)

IN625 after exposure to steam at 670 °C for 293 hrs. at 1 bar (a) and 267 bar (b). The 1 bar scale was chromia; the 267 bar scale had a metal content similar to the alloy. The marker is 50 µm.

Joining of Advanced High-Temperature Materials

Performer: Pacific Northwest National Laboratory (PNNL)

Award Number: FWP-12461

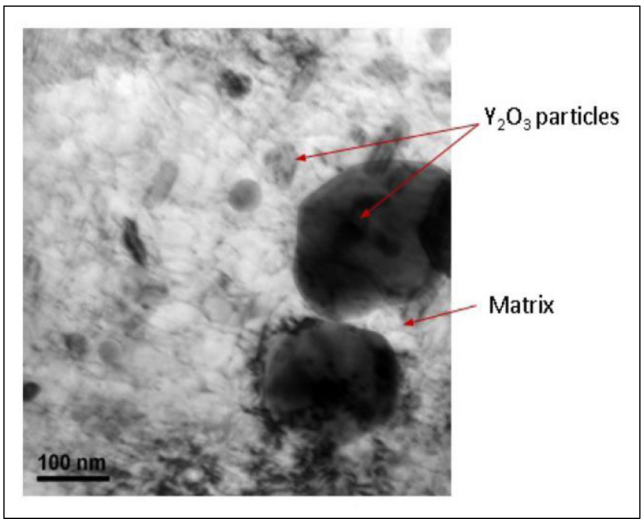
Project Duration: 10/01/1996–09/30/2014

Total Project Value: $8,315,000

Funding Source: Plant Optimization Technologies

NETL is partnering with Pacific Northwest National Laboratory to investigate the use of friction stir welding (FSW) as an alternative solid-state joining for joining pipe and tubes. This project will initially focus on three main tasks comprising (1) a parametric study to determine process parameters (i.e., spindle rotational and travel speeds, plunge force, and pin diameter/shoulder geometry) that yield defect-free welds in oxide dispersion strengthened (ODS) and other creep resistant superalloy materials; (2) mechanical and creep testing of FSW samples welded under optimized conditions; and (3) oxidation and corrosion of FSW material. As part of the latter two tasks, the research team will also perform tests on an equivalent series of specimens fabricated from the unwelded base material.

The goal of this project is to contribute to the development of cost-effective methods of joining high-performance alloys for use in advanced coal-fired power generation plants. The project will initially focus on ODS steels and Ni-based superalloys that are susceptible to sensitization upon fusion welding, with the objective of achieving joints that exhibit high-temperature strength, creep resistance, and corrosion resistance properties equivalent to the base material. Specifically, researchers will develop linear and rotary friction stir welding processes to meet this objective. Effective joining methods to maintain the material performance of high-performance alloys will enable the use of such alloys in high-temperature, high-pressure, corrosive environments including AUSC steam turbines and boilers.



TEM image of the FSW nugget in Eurofer 97 – exhibits little difference from the base metal.

An Integrated Study on a Novel High Temperature High Entropy Alloy

Performer: Southern University and A&M College

Award Number: FE0011550

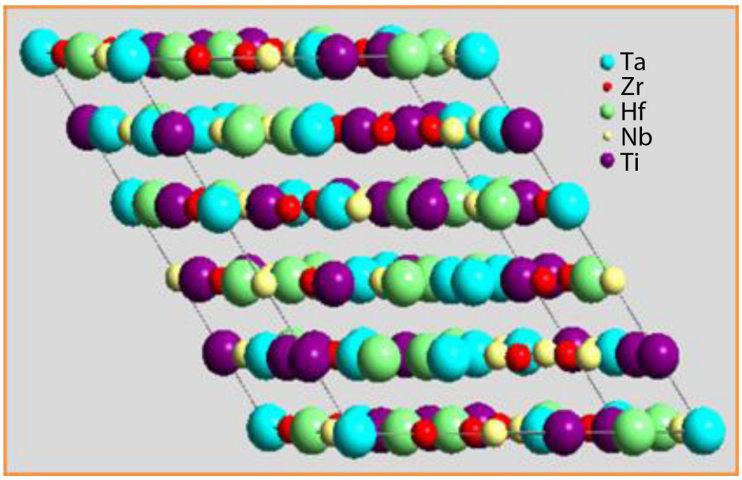
Project Duration: 10/1/2013–9/30/2015

Total Project Value: $200,000

Funding Source: 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.

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

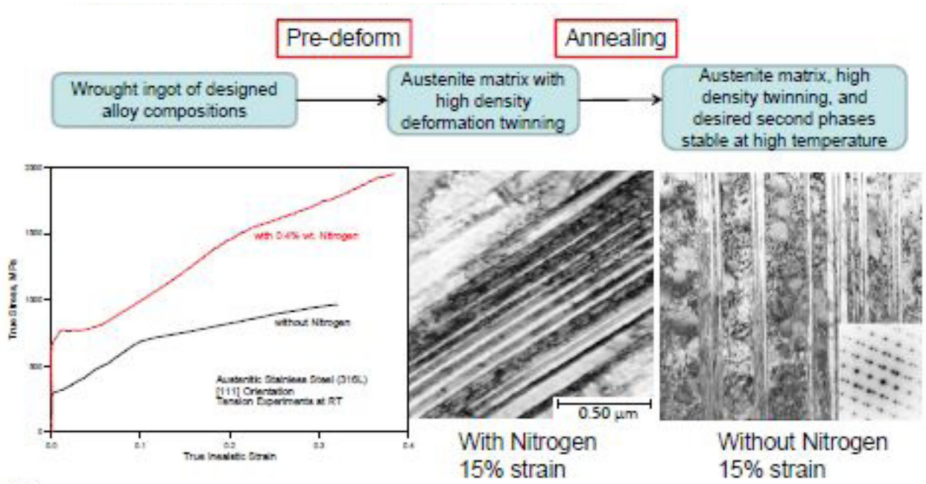
Total Project Value: $300,000

Funding Source: University Training and Research

This project will work 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 an alloying element or elements, 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.

Both microstructural design and computational alloy design will be included. In the microstructural part, effort will be devoted to create microstructures with homogeneously distributed nano-precipitates (carbides, nitrides, carbonitrides, and intermetallics) formed at high temperatures (950 ˚C and above), and intense density of low energy [high angle, low coincident side lattice (CSL)] 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 first utilized to reveal the relation between the active deformation mechanisms, mechanical performance, and microstructure features such as twinning, crystallographic texture, and precipitates. The knowledge base gained in these studies will then be used as part of the guideline for computational alloy design. After the new composition is created, thermo-mechanical processing and a twinning-induced grain boundary engineering route will be optimized for the desired microstructure. Eventually, the resulting microstructure will be characterized as well as the high-temperature mechanical properties. In the computational design part, 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. Effort will also be devoted to optimizing the heat-treatment parameters for desired microstructures, utilizing the latest thermodynamic database. The synergistic use of computational and microstructure design methods can potentially be applied to other alloy design problems.

The development of advanced, next-generation high-temperature stainless steels will enable the deployment of significantly more efficient advanced coal power generation plants.



Simple thermo-mechanical processing.

Serration Behavior of High-Entropy Alloys

Performer: University of Illinois

Award Number: FE0011194

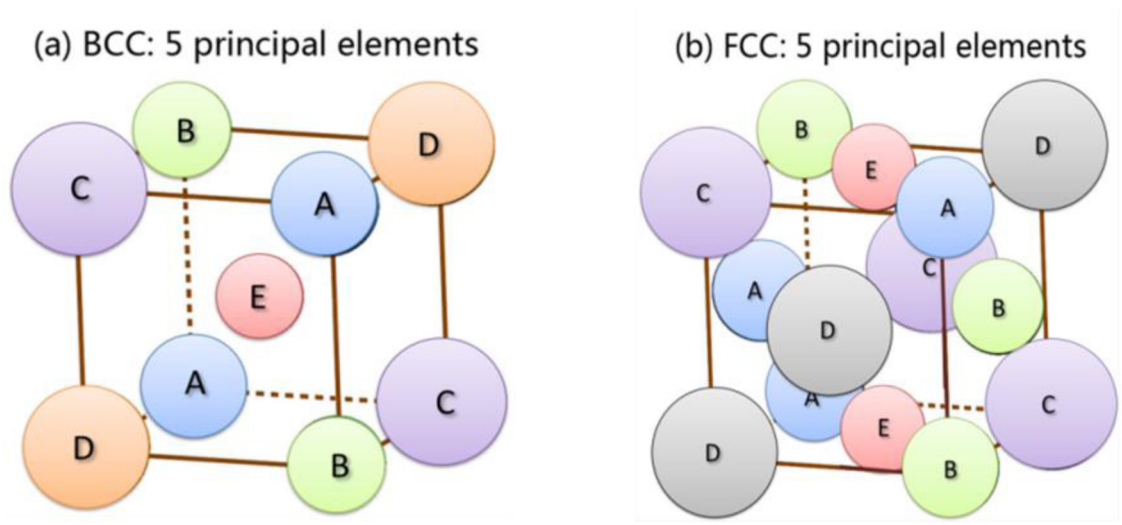
Project Duration: 10/1/2013 – 9/30/2016

Total Project Value: $300,000

Funding Source: 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 Microstructural Optimization Design Tool for High Temperature Structural Materials

Performer: University of North Texas

Award Number: FE0008648

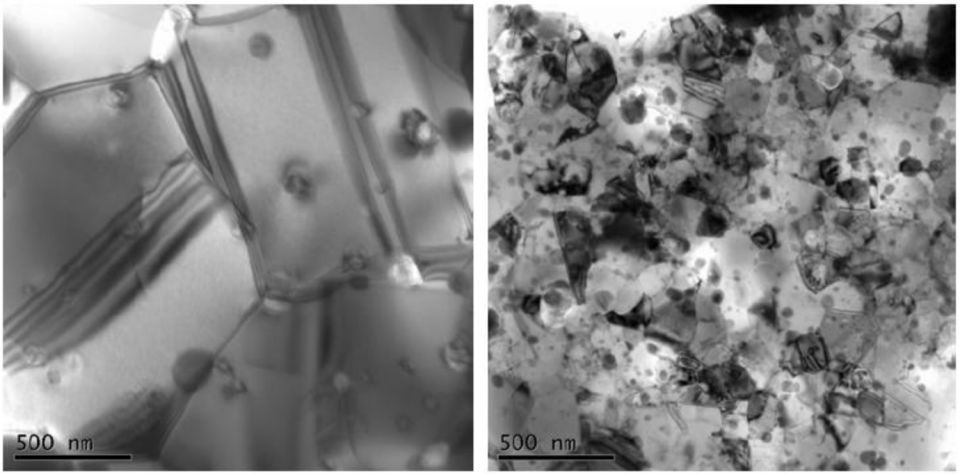
Project Duration: 9/1/2012–8/31/2014

Total Project Value: $300,000

Funding Source: University Training and Research

NETL is partnering 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 combination of high stiffness and high creep strength in an oxygen-rich and hydrogen-rich high-pressure environment. The objectives of the research project are 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.

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. The project results will lead to the development of high temperature nickel based alloys for ultra-supercritical fossil-fueled power plants.



TEM bright field images of SPSed (a) Ni-20Cr and (b) Ni-20Cr-1.2Y_2O_3 alloys.

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

Performer: University of Tennessee

Award Number: FE0005868

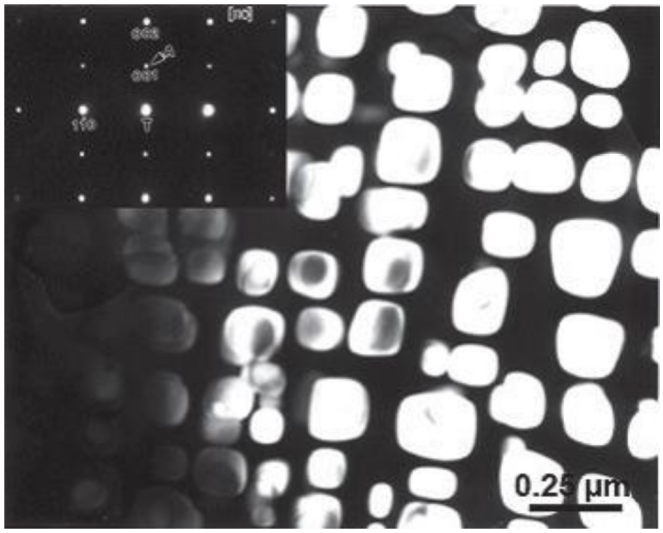
Project Duration: 10/01/2011–12/31/2014

Total Project Value: $1,508,500

Funding Source: Plant Optimization Technologies

NETL is working 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 will address this concern by targeting the development of computational tools required to design and optimize ferritic superalloys. These tools will be 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 will allow researchers to gain an understanding of the creep behavior of these high-temperature alloys.

The goal of this project is 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 will facilitate progress toward improved materials and computational modeling of these materials to permit their future implementation 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).

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

Performer: University of Texas at El Paso

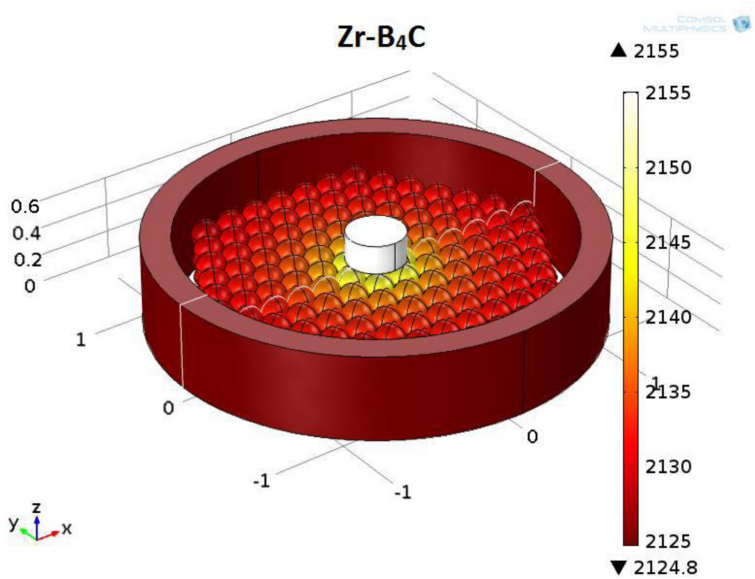
Award Number: FE0008400

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

Total Project Value: $200,000

Funding Source: University Training and Research

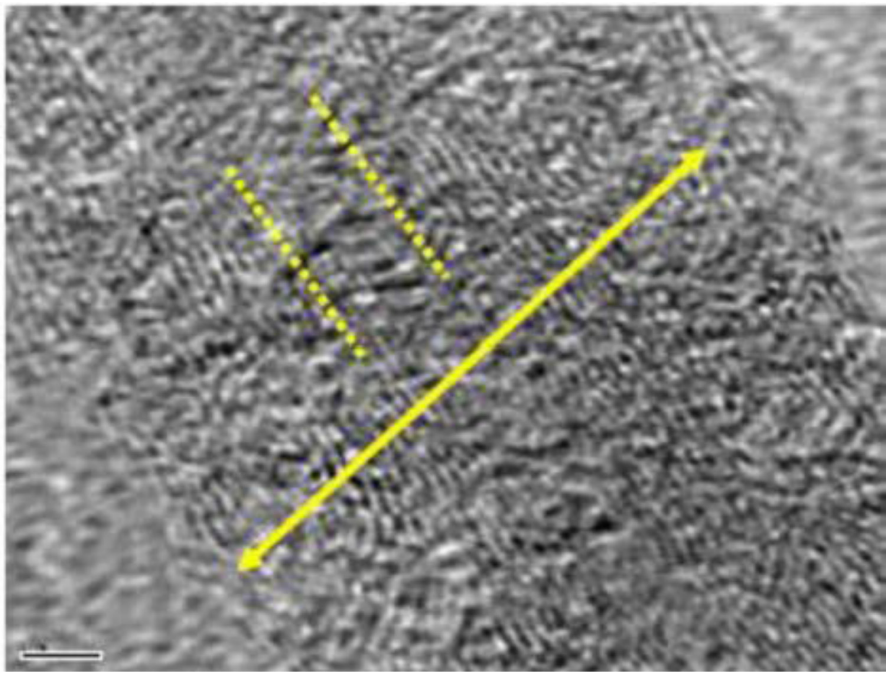
NETL is partnering with the University of Texas El Paso to investigate computationally the plasma processing with strategic experimentation of SiC, ZrC-TiC-Y_2O_3 and Ti_2AlC-TiC-Y_2O_3 packed beds, which ultimately will form SiO_2, ZrO_2-TiO_2- Y_2O_3, and Al_2O_3-Al_2TiO_5-Y_2O_3 scales for high temperature 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®.

Functional Materials

The objective of the Functional Materials research area is to understand the special requirements of materials intended to function in specific conditions such as those encountered in hot gas filtration, gas separation, and fuel cell systems.



Performer	Project Title	Page
University of Tennessee	Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage	35
University of Washington	High Temperature Thermoelectric Oxides Engineered at Multiple Length Scales for Energy Harvesting	36

Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage

Performer: University of Tennessee

Award Number: FE0011585

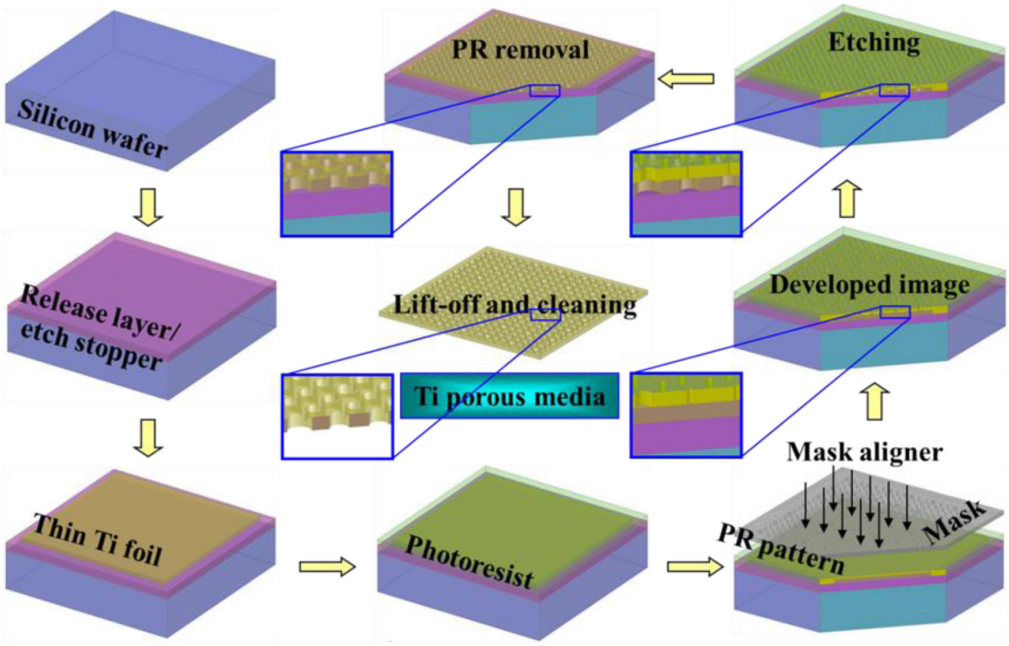
Project Duration: 9/1/2013 – 8/31/2016

Total Project Value: $470,084

Funding Source: University Training and Research

NETL is partnering with University of Tennessee to develop a thin and well-tunable multifunctional component liquid/gas diffusion layer material with micro/nano fabrication for high-efficiency electrical energy storage, which is critical for long-term coal energy applications to provide reliable, affordable electricity, and to enable electrical grid modernization. Project goals will be accomplished with modeling, a fabrication study with thin titanium foils, titanium liquid/gas diffusion layer transport enhancement and surface treatment, and comprehensive ex-situ/in-situ characterizations and tests; including the electrolyzer tests of performance and efficiency and 500-hour durability.

The successful development will make much thinner and more controllable multifunctional materials with lower flow/interfacial resistance and higher thermal/electric conductivities, thus significantly improving efficiencies of the electrolyzer or other associated energy storage devices.



Fabrication of Ti LGDLs from thin Ti films.

High Temperature Thermoelectric Oxides Engineered at Multiple Length Scales for Energy Harvesting

Performer: University of Washington

Award Number: FE0007272

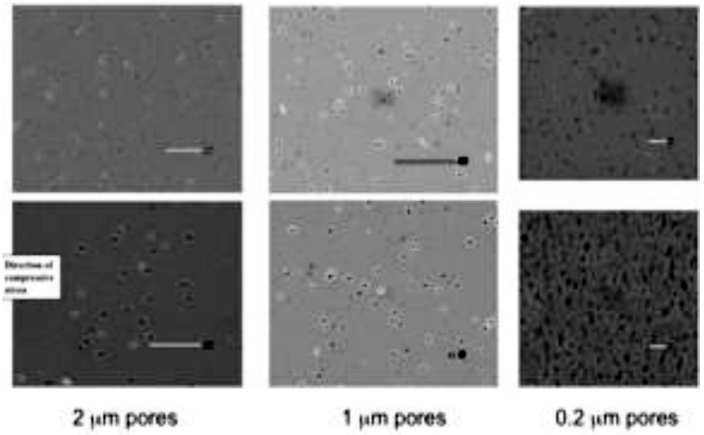
Project Duration: 9/21/2011–9/20/2014

Total Project Value: $299,956

Funding Source: University Training and Research

NETL is partnering with University of Washington to explore a novel class of 'n' type thermoelectric oxides that are stable at high temperature in the coal-fired flue gas environment. It will focus on thermoelectric oxides with high figures of merit, employing the recent observation in the literature that thermoelectric figure of merit increases rapidly in the vicinity of the Curie temperature for ferroelectric materials (thermoelectric-ferroelectric coupling). The specific objectives are: (1) to use combinatorial materials exploration to rapidly screen a broad composition range in order to identify the most promising compositions of ferroelectric materials with high Curie temperatures; (2) to investigate the thermoelectric properties of the most promising 'n' type thermoelectric oxides in these families; (3) to develop processing approaches to make oriented crystalline oxides (in order to exploit the expected anisotropic nature of the materials); and (4) to develop processing approaches to make hierarchical anisotropic porous structures in order to evaluate the effect of micro- and macro-pores on thermoelectric properties.

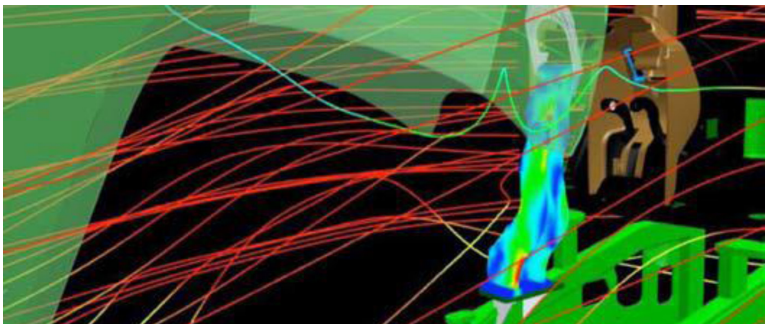
This project's success will pave the way for the development of efficient high-temperature, stable thermoelectric modules for waste heat recovery from coal-fired power plants and other industrial systems where process heat is an important byproduct (e.g., steel plants), resulting in higher efficiencies and reduced pollution and greenhouse gases. Another important outcome is the training and education of a PhD student who will work on the scientific issues outlined in the research and will also be exposed to the broader context of research in this important area of energy efficiency and security.



Powders of optimal compositions (determined by the Combinatorial Materials Exploration process) are sinter-forged to make textured bulk polycrystals. The team uses pore formers and partial sintering to create hierarchical porosity thermoelectric oxides.

Breakthrough Concepts

The objective of the Breakthrough Concepts research area is to explore routes for the development of materials with temperature/strength capabilities beyond those currently available.



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Improved Atomization Processing for Fossil Energy Applications

Performer: Ames National Laboratory

Award Number: FWP-AL-99-501-032

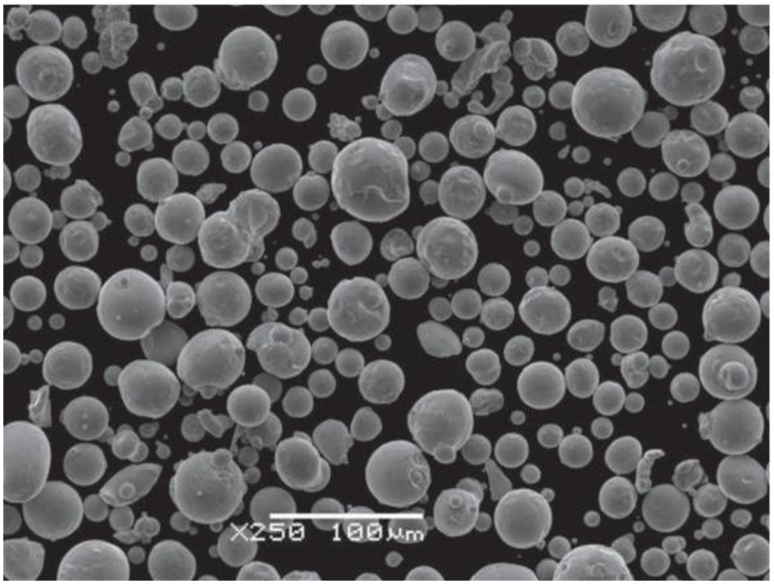
Project Duration: 10/01/1998–09/30/2014

Total Project Value: $1,564,000

Funding Source: Plant Optimization Technologies

NETL is partnering with Ames Laboratory to develop a close-coupled atomization nozzle and control system that can be calibrated to generate liquid droplets in the atomization spray, which then solidify to the specified size range of particles in powders for specific applications. Researchers will improve the design of high-efficiency gas atomization nozzles in order to maximize powder yields in special size classes most suitable for thermal-sprayed coatings. Sizes will include ultrafine powders with particle diameters of less than 10 microns (µm) and mid-range powders with particle diameters between 10 and 44 µm. Researchers will perform a detailed analysis of atomization process responses to alloy and parameter modifications to verify the effect of process innovations. The objective of this study is to design and develop metallic filters having uniform, closely controlled porosity using a unique spherical powder processing and sintering technique. The corrosion resistance of the filter materials will be evaluated under simulated pressurized fluidized bed combustion (PFBC)/integrated gasification combined cycle (IGCC) gaseous environments in order to determine the optimum alloy composition and filter structure. The corrosion tests will also provide a means to estimate the service lives of experimental filter materials when subjected to either normal or abnormal PFBC/IGCC plant operating conditions.

The goal of the project is to enable cost-efficient production and widespread use of metal powders by developing a nozzle and control system for gas atomization that can be calibrated to produce specified particle size ranges. The resulting alloys will be used in applications including coal gasifiers, heat exchangers, and gas turbine blades. Further development of other metals may be performed to fabricate components such as hydrogen separation membranes. These developments will enable more efficient power plants operating with reduced emissions and greater adaptability to carbon sequestration or capture.



Atomized powder.

Materials Research for Coal Conversion and Utilization Processes—Development of Nondestructive Evaluation (NDE) Methods for Structural and Functional Materials

Performer: Argonne National Laboratory (ANL)

Award Number: FWP 49943

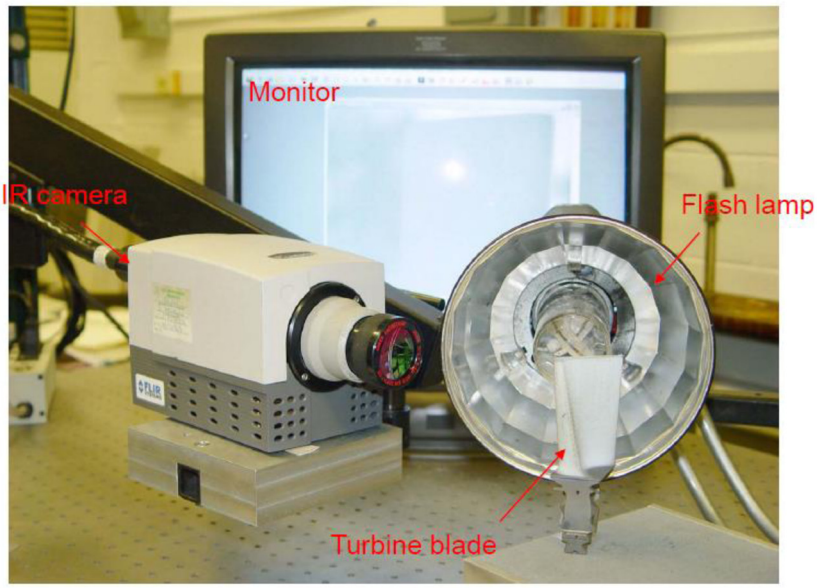
Project Duration: 10/01/2011–09/30/2015

Total Project Value: $525,000

Funding Source: Plant Optimization Technologies

The nondestructive evaluation (NDE) development is currently focused on thermal barrier coatings (TBCs) for advanced gas turbines and for high-temperature gas [(oxygen (O_2) and hydrogen (H_2)] separation membranes. Reliable NDE technologies are being developed to provide data that can be used to assess TBC conditions and predict TBC failure. This is critical, especially as TBCs have become prime reliant materials for turbine components. ANL has been developing both laser-based optical methods and one-sided infrared thermal imaging methods. In the second area, (high-temperature) O_2 and H_2 separation membranes, the NDE method under study for leak detection has been high-spatial-resolution synchrotron X-ray radiation imaging. Synchrotron microtomographs have also been evaluated to study the microstructure of membrane substrates. In addition, work has been directed on NDE detection of defects in membrane components.

The approach used for all aspects of this project is to work closely with industrial counterparts and other national laboratories that are developing new materials systems, as well as with other DOE contractors focusing on specific areas of interest. Direct interaction with universities is also part of the approach. Specific test samples are prepared by industrial and academic partners with known or intended variations in mechanical or physical properties.



One-sided flash thermal imaging setup for testing TBC-coated turbine blade.

High Resolution Modeling of Materials for High Temperature Service

Performer: Carnegie Mellon University

Award Number: FE0003840

Project Duration: 07/01/2010–06/30/2013

Total Project Value: $298,191

Funding Source: University Training and Research

NETL partnered with Carnegie Mellon University to develop new software and computational tools that will help materials developers and engineers rapidly evaluate how variations in the microstructure of metal alloys will impact the mechanical behavior of those alloys at high temperatures. The project team focused on the simulation of permanent deformation due to significant stress and damage accumulation. The approach to modeling included both three-dimensional (3-D) microstructure generation from microscopy data and an image-based method for high resolution simulation of mechanical response. The image-based simulation method used an existing 3-D fast Fourier transform (FFT)-based algorithm and extend it to compute large images using high performance computing methods. The developed models were applied to conditions where the interaction between particles and plastic deformation, whether at room temperature or under creep conditions, is critical to performance.

The goal of this project was to develop high-resolution methods for modeling the 3-D mechanical response of metallic alloys when exposed to high temperatures. The expected results of the project are new software and computational tools that will allow materials developers and engineers to rapidly evaluate how variations in the designed microstructure of metal alloys will impact the mechanical behavior of such materials at high temperatures. By reducing the time required for material analysis and selection, faster development of cleaner and more efficient fossil energy-based power generation technologies will be achieved.

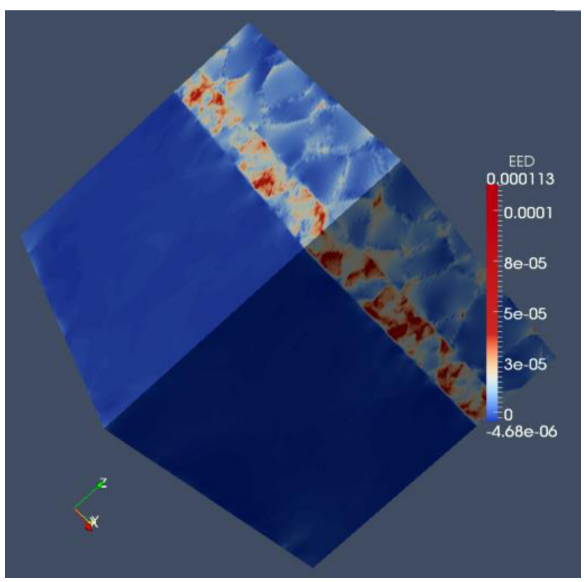


Illustration of the elastic energy density calculated for a synthetic three-dimensional microstructure that represents a layered composite material that has been subjected to a 1000 °C temperature increase (relative to a stress-free state).

Computational Capabilities for Predictions of Interactions at the Grain Boundary of Refractory Alloys

Performer: CFD Research Corporation

Award Number: FE0005867

Project Duration: 10/01/2010 – 09/30/2013

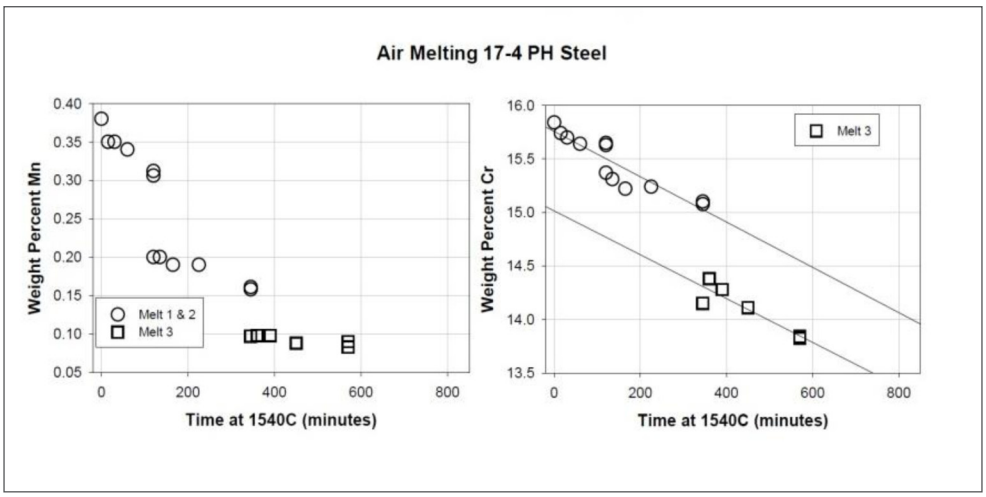
Total Project Value: $1,249,996

Funding Source: Plant Optimization Technologies

NETL partnered with CFD Research Corporation and Pennsylvania State University to further investigate—through development, demonstration, and validation of computational capabilities—the interactions at the grain boundary of refractory alloys currently being developed to withstand the high temperatures, pressures, and corrosive environments of advanced power plants. The researchers developed and validated ReaxFF (computational molecular dynamics) potentials capable of naturally accounting for various types of grain boundaries and segregants (substitutional and interstitial) that offer a compromise between high-level QM description and computational speed. This project will demonstrated the feasibility of the approach for analyzing alumina (Al_2O_3)-based refractory degradation at grain boundaries by evaluating predictions using existing ReaxFF potentials.

The overall goal of the proposed project was to provide a capability to assess degradation mechanisms and improve the reliability of refractory alloys for coal gasification and related processes.

The anticipated impact of the project is significant: accelerated development of new materials that can improve the efficiency of fossil fuel systems. Computer-aided development of materials will significantly accelerate time-to-market for new, economically viable materials for use in fossil fuel systems.



Effects of minor alloying elements.

Multiscale Modeling of Grain Boundary Segregation and Embrittlement in Tungsten for Mechanistic Design of Alloys for Coal Fired Plants

Performer: Clemson University

Award Number: FE0003892

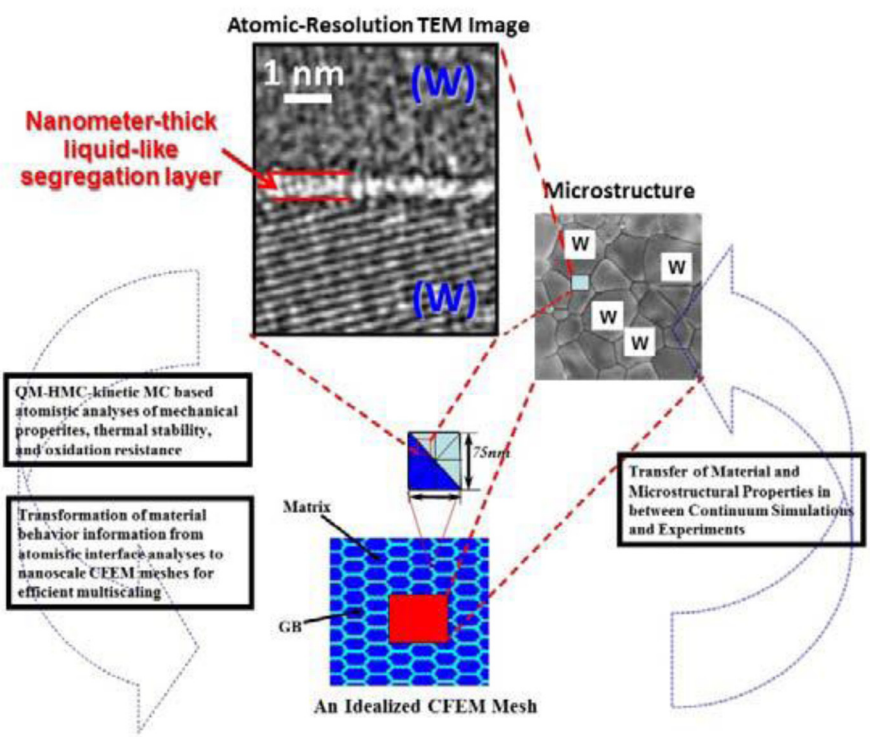
Project Duration: 07/01/2010–6/30/2013

Total Project Value: $328,196

Funding Source: University Training and Research

NETL partnered with Clemson and Purdue Universities in a project that predicts grain boundary segregation and embrittlement of alloys for use in coal-fired plants. This project investigated grain boundary segregation and embrittlement in modeled systems. The modeled systems for this project were nickel (Ni) doped tungsten (W) and Ni+X co-doped [where X = copper (Cu), cobalt (Co), iron (Fe), palladium (Pd), carbon (C), and sulfur (S)]. Project personnel developed thermodynamic theories and statistical models to compute the grain boundary diagrams of the model systems in order to link grain boundary segregation with grain boundary embrittlement. The models were validated by experiments conducted by the researchers.

The project developed a quantitative model for predicting grain boundary segregation in refractory alloys. Researchers utilized this model to develop a multiscale modeling strategy to predict grain boundary embrittlement from grain boundary segregation. This project made progress toward providing improved materials and materials modeling to allow for implementation in fossil energy conversion technologies.



A pictorial representation of the multiscale modeling approach.

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

Performer: General Electric Global Research

Award Number: FE0005859

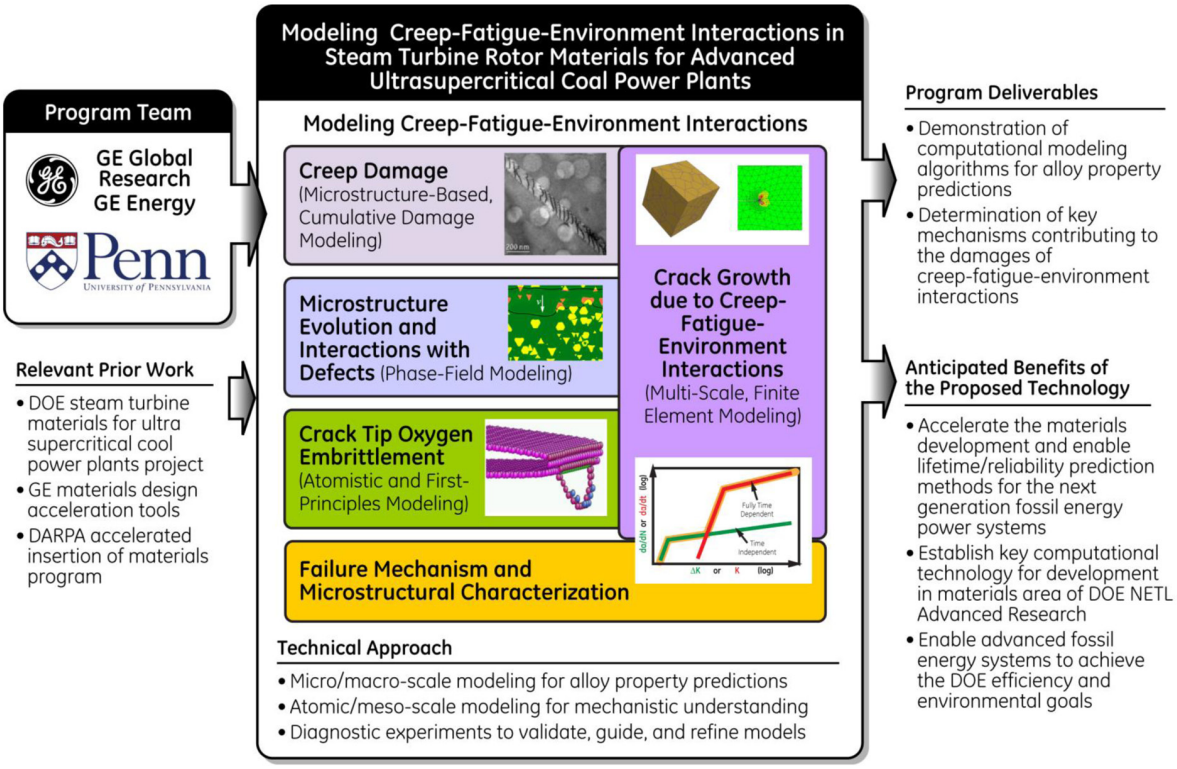
Project Duration: 01/21/2011–01/20/2014

Total Project Value: $1,499,928

Funding Source: 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 builds 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 goal of this project was to model creep-fatigue-environment interactions in steam turbine rotor materials for AUSC coal power plants, develop and demonstrate computational algorithms for alloy property predictions, and determine and model 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.



Model Creep-Fatigue-Environment Interactions in Steam Turbine Rotor Materials for Ultrasupercritical Coal Power Plants.

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

Performer: Howard University

Award Number: FE0011515

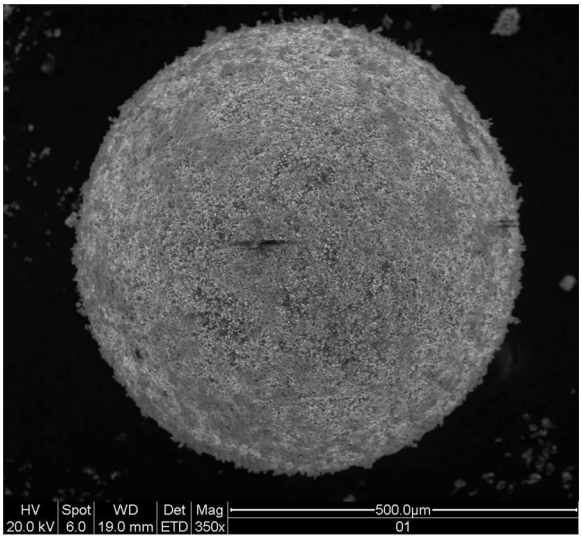
Project Duration: 7/1/2013–6/30/2015

Total Project Value: $199,892

Funding Source: University Training and Research

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, 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.

Computational Materials – Integrated Materials Initiative

Performer: National Energy Technology Laboratory Office of Research and Development

Award Number: IPT_FY14

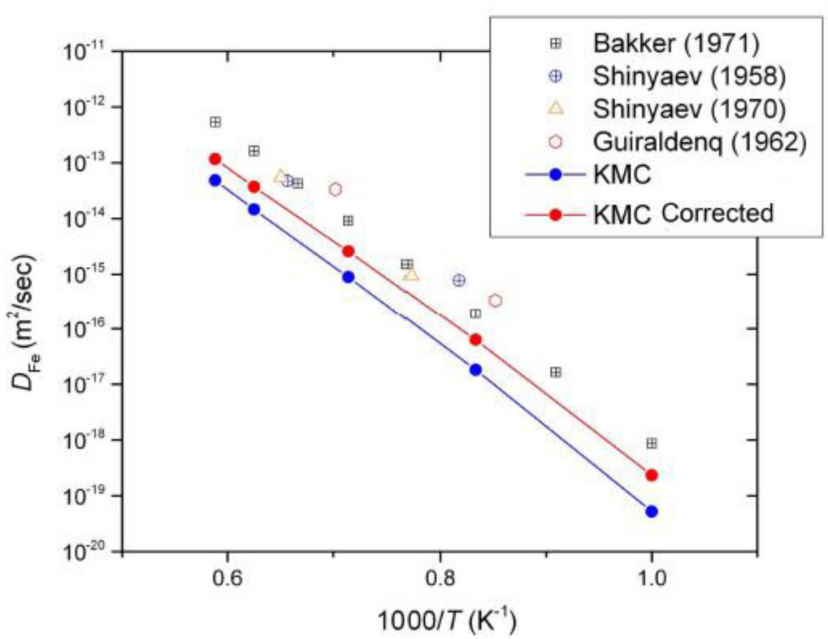
Project Duration: 10/01/2013-9/30/2014

Total Project Value: $1,304,000

Funding Source: Plant Optimization Technologies

This project will develop and validate computational atomistic simulations for key variables and parameters required for the microkinetic model to predict oxidation behavior of alloys. 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 operating capital and operating costs. Specifically this project will evaluate the influence of ambient gases (O_2, H_2, H_2O, and CO_2) to predict the influence on alloy surfaces.

Advanced fossil fueled power systems, such as A-USC or oxyfuel combustion systems, require cost effective materials of construction that can withstand the extreme (mechanical and corrosive) environment for 10,000 to 100,000 hours. The ultimate goal of the computational materials task is to develop a series of validated multi-scale computational toolsets that reduce the timeline for the identification and development of cost effective materials for advanced energy systems. Current work is focused on developing a microkinetic model to predict alloy compositions necessary to form stable oxide scales when exposed to extreme environments; implementation and validation of the microkinetic model (for Ni-Fe-Al alloys); developing a tool set to predict service life of alloys (oxidation kinetics) for alloys exposed to extreme environments; and developing models to assess the impact of microstructural stability on key high-temperature strengthening mechanisms in alloys for application in advanced energy systems.



The predicted diffusivity of Al in Ni (dilute concentration; x=0.1% Al) will be compared to experimental results from the literature.

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

Performer: North Carolina State University

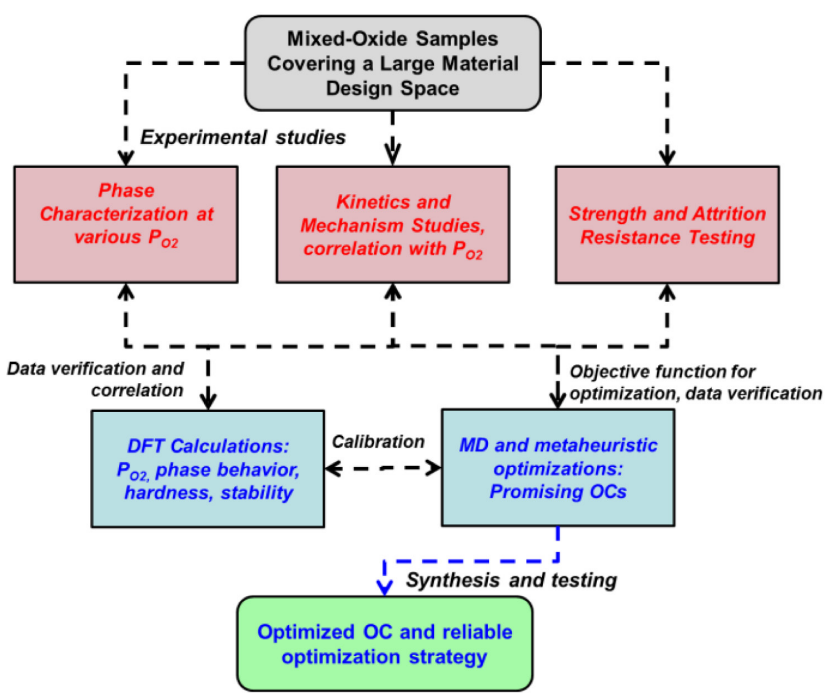
Award Number: FE0011247

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

Total Project Value: $363,404

Funding Source: 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 diffractions, 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. Accurate multi-scale simulation models and 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.

Qualification of New, Commercial Oxide Dispersion-Strengthened Alloys for Use in Advanced Fossil Processes

Performer: Oak Ridge National Laboratory

Award Number: FWP-FEAA109

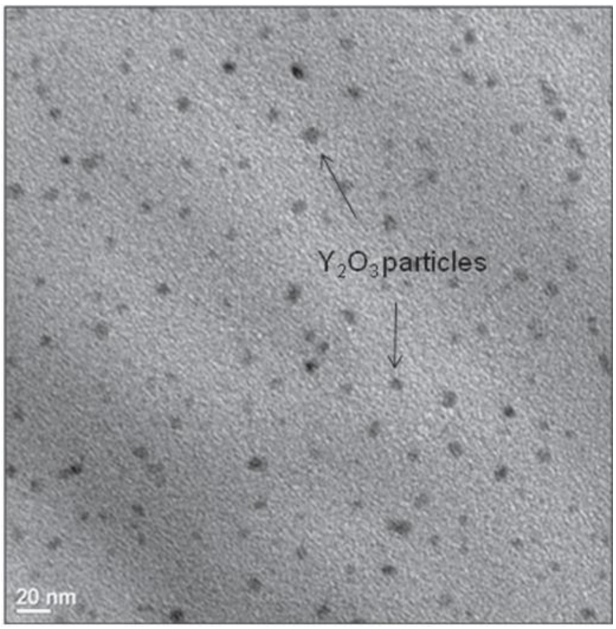
Project Duration: 10/01/2009–09/30/2014

Total Project Value: $1,862,500

Funding Source: Plant Optimization Technologies

DOE NETL is supporting an effort by Oak Ridge National Laboratory to characterize Dour Metal's key products (ODM 751 and ODM 401) for use in DOE's advanced power generation processes. The project will produce a set of data sheets that provide physical, chemical, and mechanical properties for use by equipment manufacturers considering oxide dispersion-strengthened (ODS) steels as a material option for the manufacture of advanced components. Additionally, a technology transfer workshop will be planned to provide an update on the status of ODS alloys including availability, properties, and current capabilities for fabrication of components.

The purpose of this task is to determine the capabilities of new, commercially-produced ODS alloys for application at temperatures up to 1200 °C in environments associated with advanced fossil combustion and conversion processes. These advanced processes will have higher efficiencies, require less fuel input, and ultimately produce less carbon dioxide and fewer emissions. Decreased fuel demands will conserve the nation's fossil fuel resources and place less demand on the fuel delivery infrastructure, resulting in lower secondary emissions in the supply chain.



Transmission electron microscopy images of mechanically alloyed powder of ODM 751. The dispersed oxide particles are yttrium oxide (Y_2O_3).

Low Cost Fabrication of ODS Materials

Performer: Pacific Northwest National Laboratory (PNNL)

Award Number: FWP-60098

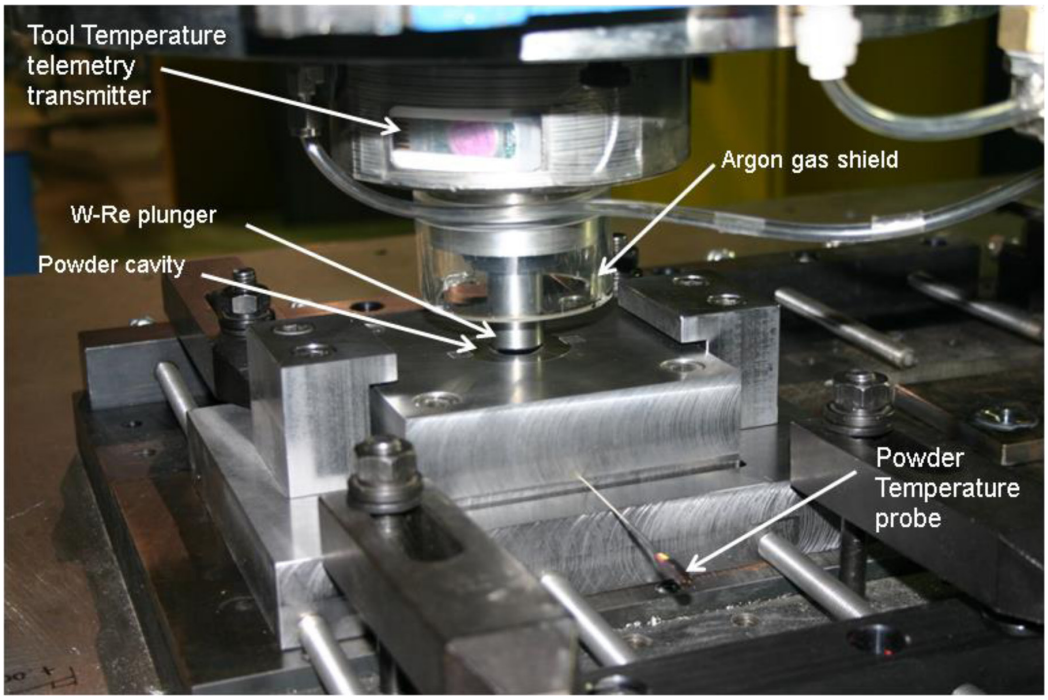
Project Duration: 10/01/2010–09/30/2014

Total Project Value: $570,000

Funding Source: 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 the barriers 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 and powder blend 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 this 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.

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

Performer: Purdue University

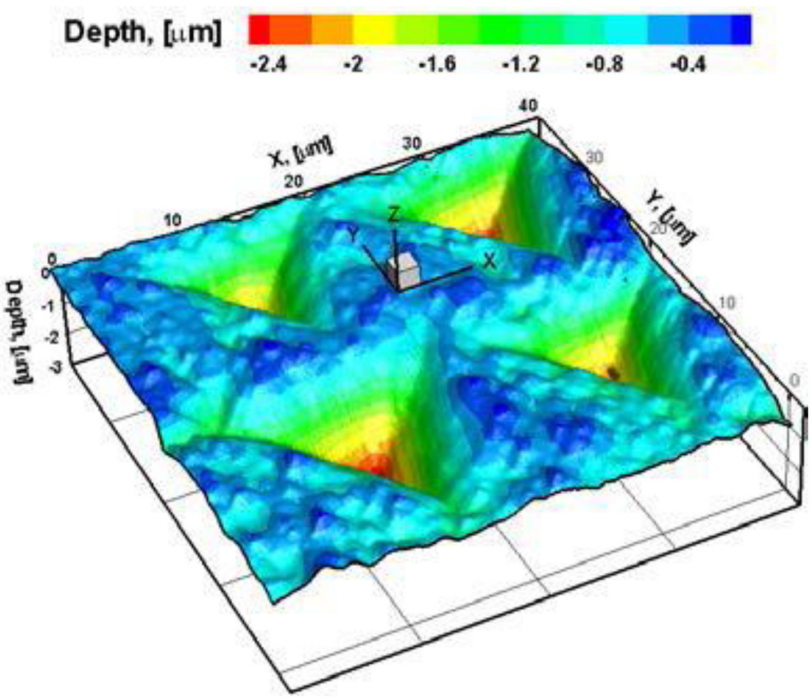
Award Number: FE0011291

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

Total Project Value: $300,000

Funding Source: 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 tungsten (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.



Scan of a sample analyzed for nano- and microscale indentation creep properties.

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

Performer: Southern University and A&M College

Award Number: FE0008382

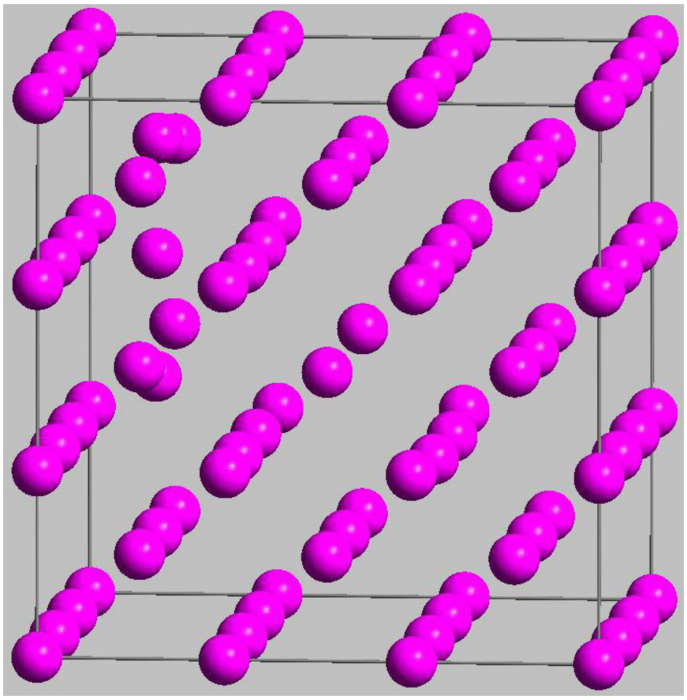
Project Duration: 6/1/2012–5/31/2015

Total Project Value: $200,000

Funding Source: 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.

Computational Studies of Physical Properties of Nb-Si Based Alloy

Performer: Tennessee State University

Award Number: FE0003798

Project Duration: 07/26/2010 – 07/31/2013

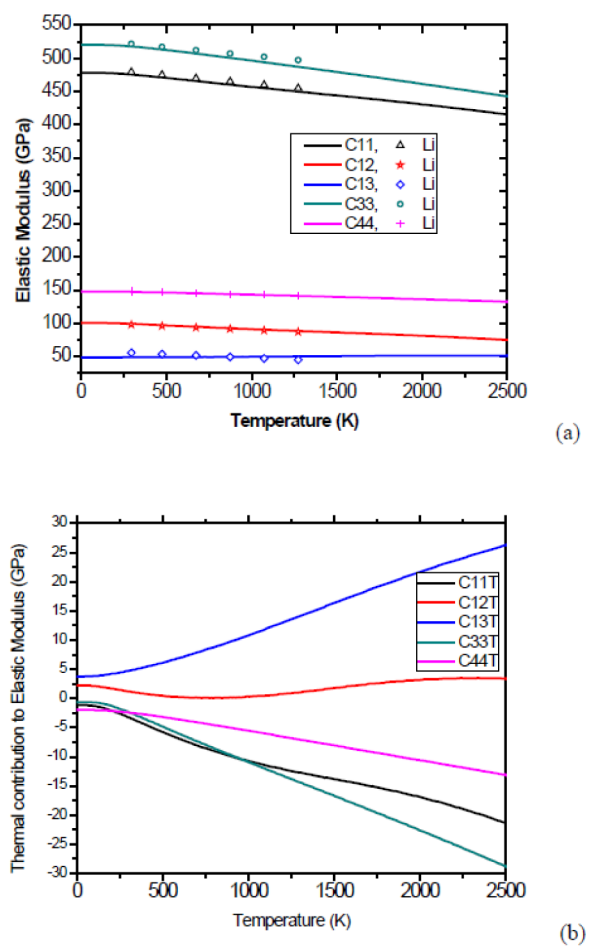
Total Project Value: $200,000

Funding Source: University Training and Research

NETL partnered with Tennessee State University to develop computer-aided material design to accelerate the development of niobium (Nb)-silicon (Si) based refractory alloys for advanced energy applications. In an effort to manage the complexity and further the development of a suitable Ni-Si based alloy, the project team provided physical properties data at first-principles calculation quality for thermodynamic modeling and other higher level simulations of these alloys. The project team further developed their Gibbs free energy package to support free energy calculations of structure types. The project team then developed an interface between the Gibbs free energy package and the popular Calculation of Phases Diagram (CALPHAD) software, Thermo-Calc®. The integrated tool was utilized to study thermodynamic properties of various phases found in Nb-Si-based alloy with a focus on the Nb-Si-chromium(Cr)-X (X=titanium (Ti), aluminum (Al), hafnium (Hf), molybdenum (Mo), etc.) system. The project also studied interfaces found in the Nb-Si-based alloys. Structural models for the interfaces among the main bulk phases, Nb solid solution, and Nb silicides were developed. Formation energies of the undoped and doped Nb-Si-Cr were calculated and compared. Interfacial mechanical properties were evaluated using similar approaches developed for ceramic interfaces.

The overall goal was to provide valuable insight into the mechanisms and processes that could lead to next-generation hot section material operating at temperatures beyond 1350 °C, which could play an important role in advancing greener energy.

Successful modeling and simulation development will lead to accelerated design and development of new materials. Development of these materials will result in the ability of coal-fired power plants to operate at desired conditions, resulting in improved efficiency and a corresponding reduction of all effluents and waste products, including carbon dioxide, an important greenhouse gas.



Temperature-dependent elastic constants of 2H-SIC at ambient pressure (a) the total elastic constants. (b) Contributions from thermal excitation and zero point energy.

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

Performer: University of Missouri – Kansas City

Award Number: FE0004007

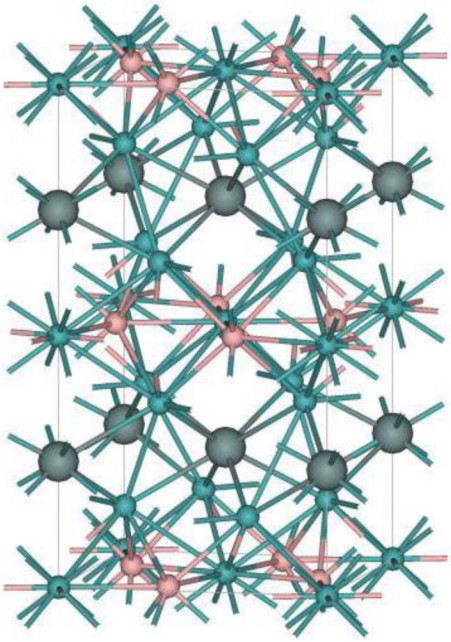
Project Duration: 07/01/2010–12/31/2013

Total Project Value: $299,925

Funding Source: University Training and Research

NETL partnered with the University of Missouri–Kansas City in a project that researched and developed new molybdenum (Mo)-based materials for use in high-temperature, high-pressure environment applications in fossil energy conversion technologies. The project also developed a new computational method and related algorithms to aid in modeling these new materials. The project addressed 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 made 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

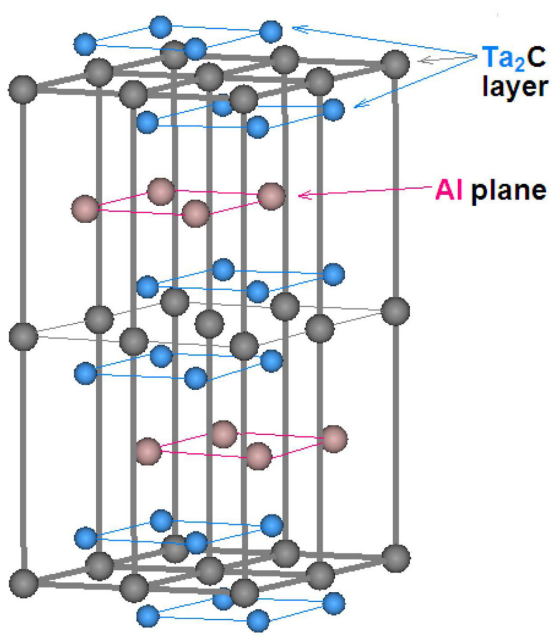
Project Duration: 08/01/2010–12/31/2014

Total Project Value: $1,127,346

Funding Source: Coal Utilization Sciences

NETL has teamed with University of Missouri–Kansas City and Tennessee State University to conduct computational studies that support the search for novel materials or significant improvements in existing materials that can meet requirements of AUSC systems. This project focuses 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 some of the most desirable properties such as damage resistance, oxidation resistance, excellent thermal and electric conductivity, machinability, and fully reversible dislocation-based deformation.

The project goal is 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 can advance the search for novel materials or lead to significant improvements to existing 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.

Mechanically Activated Combustion Synthesis of MoSi2-Based Composites

Performer: University of Texas at El Paso

Award Number: FE0008470

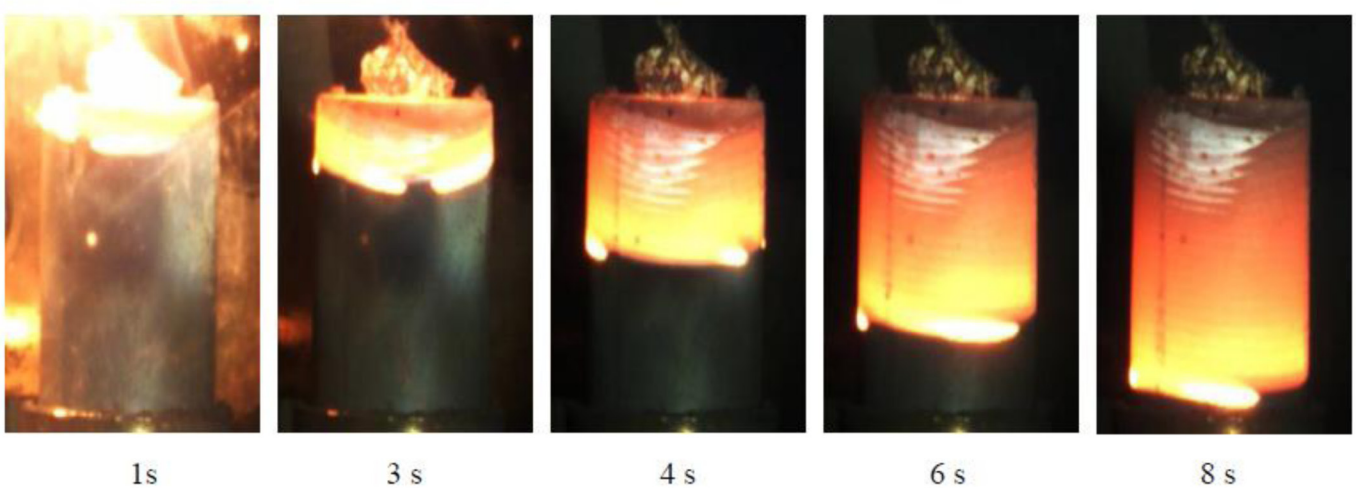
Project Duration: 7/1/2012–6/30/2015

Total Project Value: $236,000

Funding Source: University Training and Research

NETL is partnering with 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.

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

Performer: University of Toledo

Award Number: FE0008774

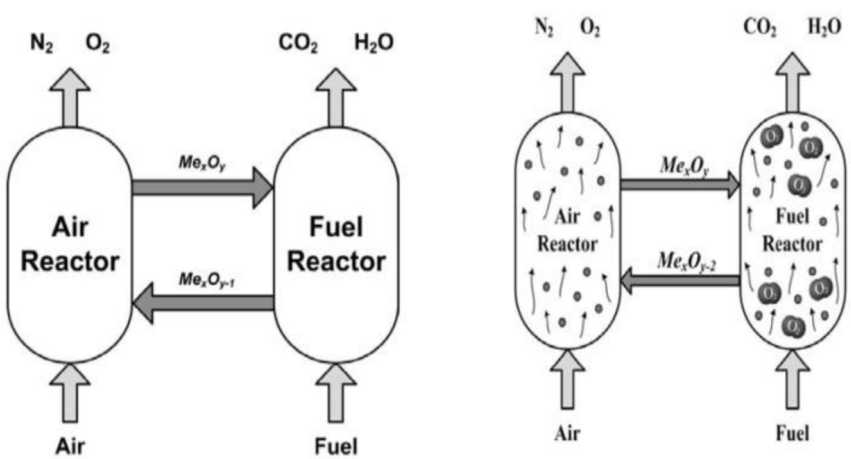
Project Duration: 9/4/2012–9/3/2016

Total Project Value: $470,674

Funding Source: 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.

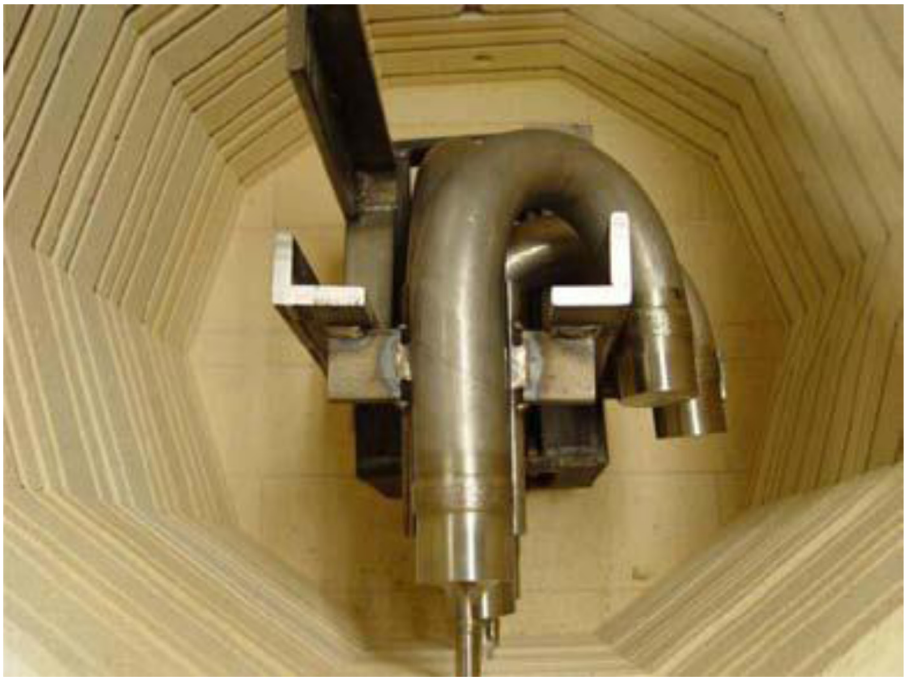
This project will develop and produce new perovskite-based oxygen carriers expected to have greater thermal and chemical stability over a wide range of temperatures and oxygen partial pressures and be environmentally safer than current materials. These new oxygen carriers may contribute to the advance 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.

Advanced Ultrasupercritical Materials

The objective of the Advanced Ultrasupercritical Materials research area is to evaluate and develop materials technologies that allow the use of advanced steam cycles in coal-based power plants to operate at steam conditions of up to 760 °C (1400 °F) and 5,000 psi.



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Development of Computational Capabilities to Predict the Corrosion Wastage of Boiler Tubes in Advanced Combustion Systems

Performer: Babcock & Wilcox

Award Number: FC26-07NT43097

Project Duration: 08/14/2007–08/31/2013

Total Project Value: $2,629,429

Funding Source: Plant Optimization Technologies

NETL collaborated with Babcock & Wilcox (B&W) on a project to develop corrosion models capable of predicting corrosion wastage (deterioration) in lower furnace walls and superheater/reheater tubes. Eight common U.S. coals were combusted in a burner flow reactor to closely simulate actual staged combustion encountered in utility boilers. Once the conditions were defined, a series of long-term (1,000-hour) laboratory corrosion tests followed. The goal of this project was to improve the performance of materials used in the construction of boilers, superheaters, and reheaters used in advanced combustion systems in order to increase their efficiency and reduce operational maintenance. The major objectives of this project were (1) to determine the effect of coal chemistry and impurities on the rate of tube corrosion at boiler operating conditions and (2) to develop two predictive equations that can be used to calculate wastage rates: one for furnace walls due to low-NO_x corrosion and the other for superheaters/reheaters due to coal ash corrosion. As a first step and in order to have the necessary data to produce the models, researchers developed a corrosion database linking materials behavior to coal chemistry.

A predictive tool to determine corrosion wastage rates in lower furnace walls and superheater/reheater tubes will aid in the design and maintenance of boilers, especially those operating at elevated temperatures, and will contribute to attainment of DOE targets for increased efficiency and reduced emissions in power plants.

Two fireside corrosion furnace facilities used for the laboratory testing: samples of ten different alloys and three weld-clad coating materials are being tested in the simulated upper furnace conditions. Samples of ten different alloys and two weld-clad coating materials are being tested in the lower furnace conditions.

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

Performer: Energy Industries of Ohio, Inc.

Award Number: FE0000234

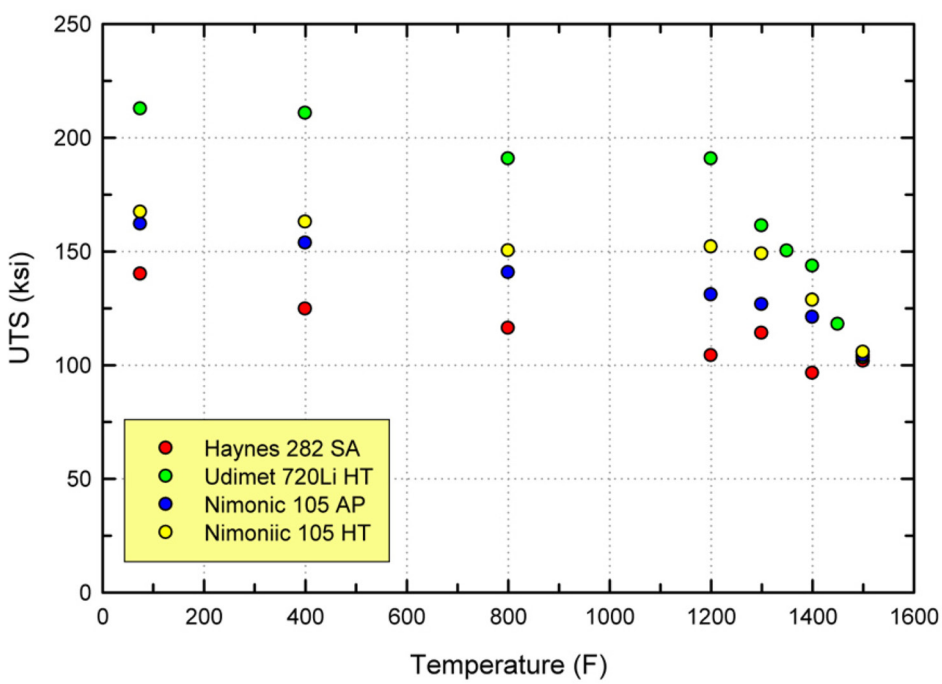
Project Duration: 10/01/2009–09/30/2014

Total Project Value: $10,800,077

Funding Source: 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 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.

Alloy Manufacturing and Process Development–Large Scale Ni-Based Alloys

Performer: National Energy Technology Laboratory Office of Research and Development

Award Number: FWP-2012.03.01

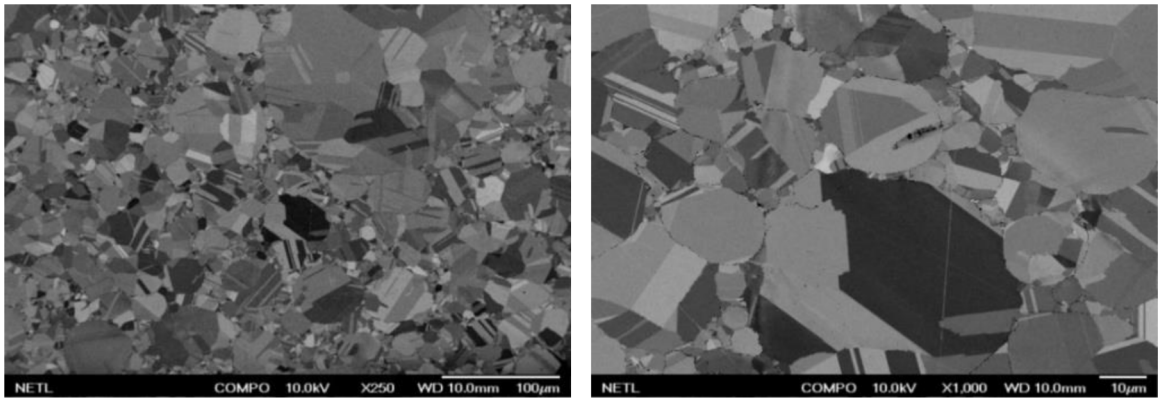
Project Duration: 10/1/2013–09/30/2014

Total Project Value: $132,000

Funding Source: Plant Optimization Technologies

The focus of this project is the development of alloys and processes that can practically be made at the scale of manufacturing deployment. The use of these alloys and processes will lead to reduced operating costs in ultrasupercritical (USC) and Advanced USC environments. Specifically, this project will include experimentation and computational studies on Ni-base alloys.

The main objective of this activity is to develop casting processes that can practically be transferred to industry. Work previously has focused on alloy design to produce nickel (Ni)-base castings and associated heat treatments to refine microstructure as well as produce peak strength. Melting, thermo-mechanical processing (TMP) and heat treatment strategies have focused on producing high quality Ni-base and steel forgings, i.e., with low levels of residual contamination (goal: clean, precisely manufactured alloys). Contacts with casting vendors, primary and secondary metal producers and OEM turbine manufacturers have been established to facilitate the supply of, and process development for, large-scale Ni-base superalloy castings for power plant application as well as high quality wrought Ni-base and steel products. Optimization and refinement of alloy homogenization procedure have progressed to the point where the desired degree of homogenization, i.e., distribution of alloy constituents within the matrix, can be achieved leading to a specified, and/or minimal (or zero), level of segregation within the cast microstructure. The minimization of sulfur in Ni-base alloys has been a priority and the path forward to reduce sulfur as well as other minor impurity elements has been established. Computational thermodynamics modeling was, and continues to be, used to determine both the critical level of sulfur in the Ni-base alloys as well as the most efficient way to achieve this level. Experimental laboratory characterization and mechanical testing has verified the computational simulations.



The spherical shape of the consolidated powder is maintained by the second phase particles outlined the powders.

Alloy Manufacturing and Process Development - Optimized Alloys for USC and A-USC Components

Performer: National Energy Technology Laboratory Office of Research and Development

Award Number: FWP-2012.03.01

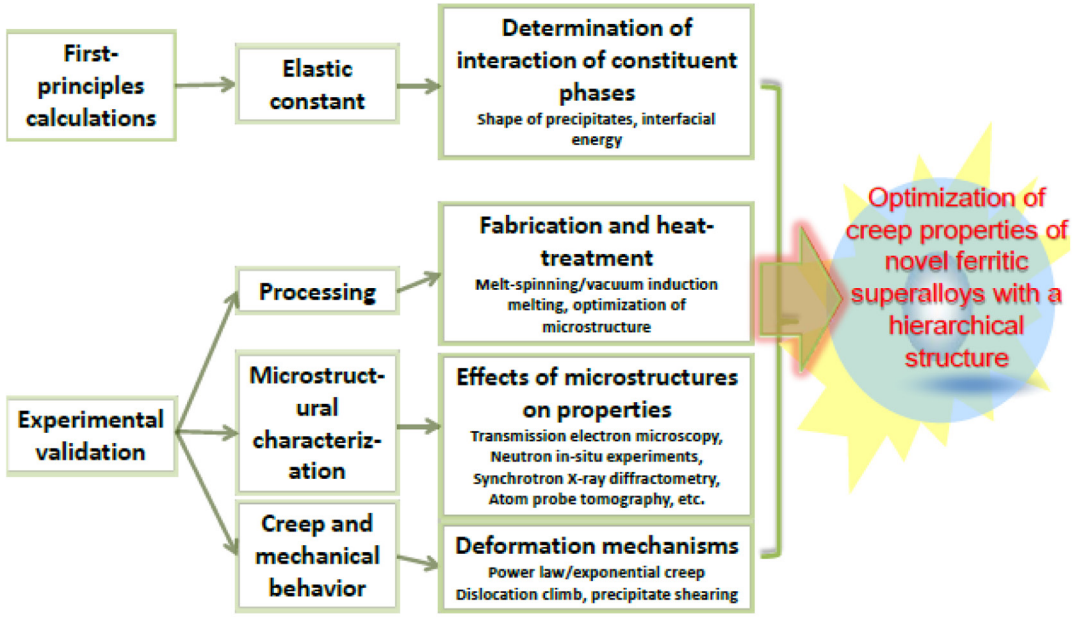
Project Duration: 10/1/2011–09/30/2014

Total Project Value: $324,000

Funding Source: Plant Optimization Technologies

The focus of this project is the development of alloys and processes that can practically be made at the scale of manufacturing deployment. The use of these alloys and processes will lead to reduced operating costs in ultrasupercritical (USC) and Advanced USC environments. Specifically, this project will include experimentation and computational studies on Ni-base alloys.

This task is to facilitate the manufacture of critical components for application in USC and A-USC boilers and steam turbines. At this point the viability of achieving 650 °C advanced 9% Cr steel for use in USC boiler and steam turbine components is being established through elevated temperature mechanical testing. The advanced 9% Cr chemistry has been determined and mechanical properties have been developed for five small laboratory heats. Within these laboratory heats variation in minor constituents and other important additions were assessed. A patent application was constructed and submitted. Creep tests (still underway) are establishing the engineering creep curves necessary for conceptual plant design. Also, computational simulations and follow up experimental castings have been completed to assess optimized γ' strengthened Ni-base formulations based on Haynes 282 for A-USC applications, in wrought product form, that lead to reduced coarsening rate for the γ' precipitate, resulting in a more stable alloy. These activities have resulted in (1) high-strength ferritic/martensitic steel with precisely controlled minor constituents for use in USC air- and oxy-combustion power plants and (2) path forward for developing a new Ni-base γ' strengthened heat resistant alloy for A-USC power plants.



Large Scale 9% Cr Steel Casting for USC 650 deg C Boiler and Steam Turbine Components

Performer: National Energy Technology Laboratory Office of Research and Development

Award Number: FWP-2012.03.01

Project Duration: 10/1/2011–09/30/2014

Total Project Value: $53,000

Funding Source: Plant Optimization Technologies

The focus of this project is the development of alloys and processes that can practically be made at the scale of manufacturing deployment. The use of these alloys and processes will lead to reduced operating costs in ultrasupercritical (USC) and Advanced USC environments. Specifically, this project will include experimentation and computational studies on Ni-base alloys.

This subtask is similar in concept to the task of casting large-scale Ni-base castings; however, several considerations will differ. As it turns out, while the Ni-base alloys solidify from start to finish with a face-centered cubic (FCC) crystal structure, the 9% Cr steels under consideration solidify about 75% of the way as body-centered cubic (BCC) then finish solidifying with an FCC crystal structure. This has a dramatic effect on the solute partitioning with some elements greatly depleted from the BCC phase and enhanced in the FCC phase or vice-versa. The segregation of each element is influenced in a complex way by the other elements in solution. As such, careful consideration of the level of each alloying element will need to be made while balancing these for oxidation resistance and strength in the final product. At the homogenization temperatures the castings will be fully FCC (with minor precipitate phases). The result of this is that diffusion will occur much more slowly. Small-scale castings will be made utilizing NETL's "enhanced" slow cooling method developed for the Ni-base alloys research. Furthermore, control of nitrogen without the formation of gas bubbles in the casting will also need to be considered. These efforts will be guided by computational thermodynamics and kinetics simulations. The effort will result in heat resistant steel casting similar in structure and properties to the current NETL advanced 9% Cr wrought steel.

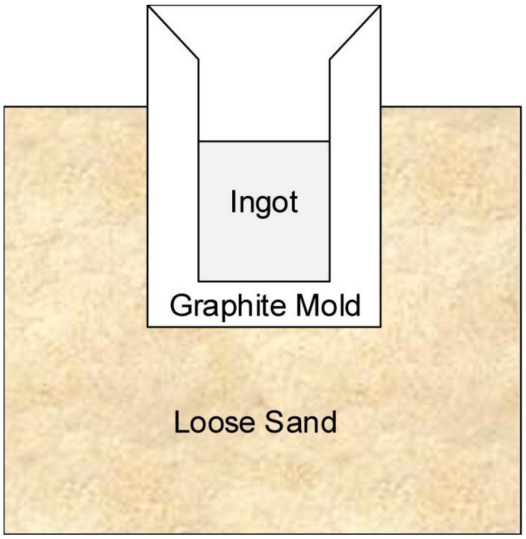


Diagram of mold submerged in loose sand to help contain heat of molten steel, thereby slowing the cooling rate substantially in order to better emulate the slow cooling conditions of a thick wall, full-size casings.

Improving the Performance of Creep-Strength Enhanced Ferritic Steels

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA107

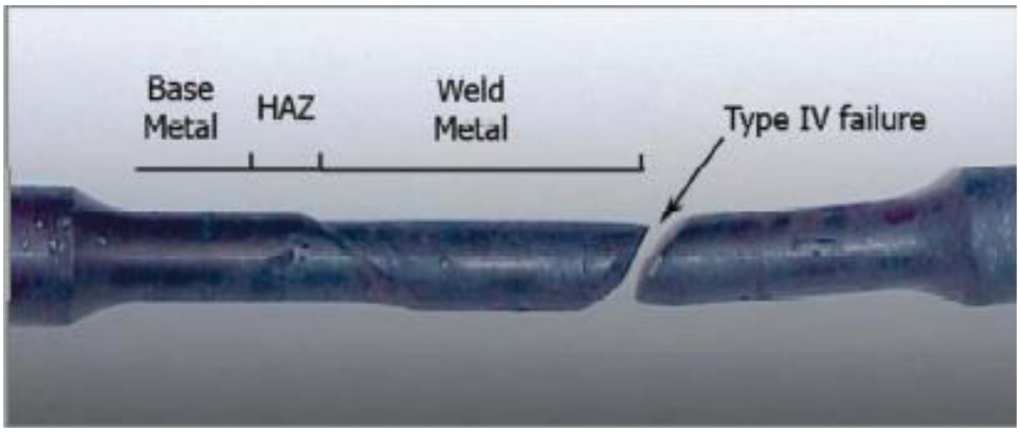
Project Duration: 10/01/2009–09/30/2014

Total Project Value: $750,000

Funding Source: Plant Optimization Technologies

NETL is partnering with ORNL to better understand how components made from creep strength-enhanced ferritic (CSEF) steels, such as alloys containing nine percent chromium (9Cr steel), fail. This project will address two broad technical issues of (1) controlling mechanical properties and microstructure, and their dependence on chemical compositions and heat treatments, and (2) understanding the causes of Type IV failure and developing strategies to minimize or eliminate it in these steels. The overall project approach will rely on fundamental and applied studies of the effects of heat treatment, welding, and process control on microstructural evolution and material properties in CSEF steels.

The goal of this program is to improve the performance of CSEF steels, with the specific objectives of providing guidelines for the maximum safe use temperatures of this class of alloys, understanding the causes of the current temperature limitations, and developing approaches for increasing the current practical use temperature limits. This project will extend our understanding of (1) an important failure mode for high-performance steels that are widely used in the power industry, (2) the conditions that lead to such failures, and (3) a means to avoid those conditions.



Type IV failure of chromium-molybdenum steel welds.

Materials for Advanced Ultrasupercritical Steam Power Plants

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA061

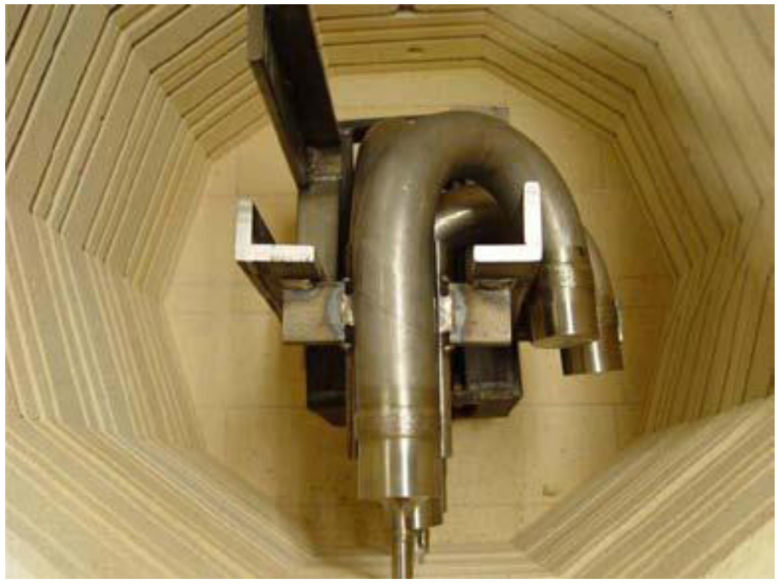
Project Duration: 09/29/2009 – 09/30/2014

Total Project Value: $1,850,000

Funding Source: Plant Optimization Technologies

This research project is integrated into the overall U.S. DOE/OCDO sponsored Advanced Ultra-supercritical (AUSC) Steam Boiler Consortium which seeks to develop the materials technology required to operate a power steam boiler at steam conditions up to 760 °C (1400 °F) 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 Bend Test Rig.

Ultrasupercritical Steam Cycle Turbine Materials

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA069

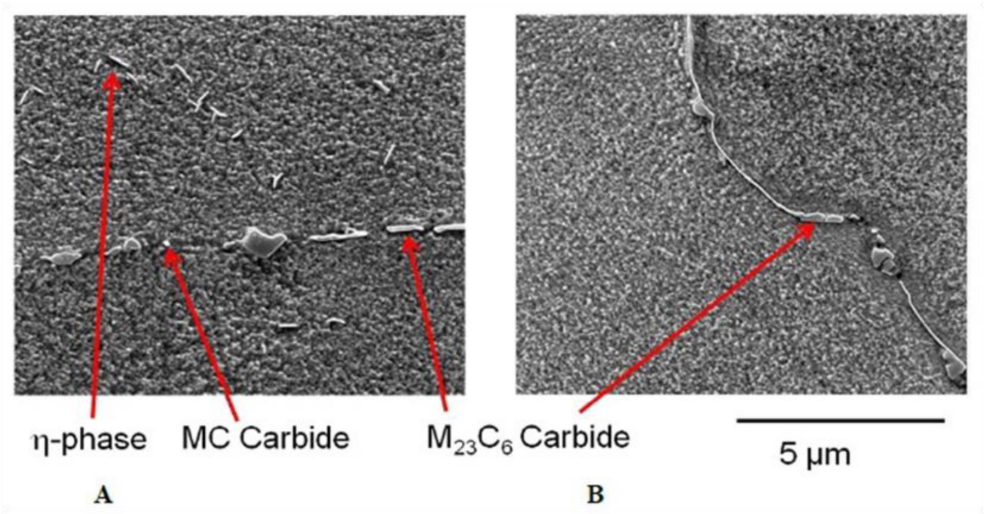
Project Duration: 10/01/2009 – 09/30/2013

Total Project Value: $500,000

Funding Source: Plant Optimization Technologies

NETL collaborated 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 used ORNL's expertise and facilities to develop methods for overcoming current materials limitations. The main areas of interest were high-temperature creep strength, corrosion behavior in steam, and weldability. ORNL researchers performed detailed evaluations to understand the potential for developing cast Ni-based alloys with improved strength and acceptable fabricability. Researchers modified 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 was 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 contributed 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]

Understanding Corrosion Mechanisms in Oxy-Fired Systems

Performer: Oak Ridge National Laboratory (ORNL)

Award Number: FWP-FEAA106

Project Duration: 10/01/2009–09/30/2014

Total Project Value: $1,425,000

Funding Source: Plant Optimization Technologies

NETL is partnering with ORNL to (1) understand temperature-relevant corrosion mechanisms, (2) determine the role of the combustion environment on the mechanical response of alloys, (3) evaluate upper temperature limits for new materials, and (4) characterize corrosion reaction products and alloy degradation of candidate high-temperature alloys and coatings in oxy-firing systems.

The primary goal of the project is to develop an improved mechanistic understanding of the role of water and carbon dioxide (CO_2), including the role of composition, on materials performance in the fireside environment of coal-fired power systems. This project will also determine the ease with which current boilers can be converted to oxy-firing systems, and the boiler components in most need of replacement with more corrosion-resistant materials. The primary benefit of this project is the creation of a knowledge base with the potential to support material selection and development for the demanding requirements of advanced, higher-efficiency steam cycles in order to reduce coal consumption and CO_2 emissions while reducing the power requirements for CO_2 capture, transport, and storage systems.

Typical components of oxy-fired system requiring materials able to withstand high-temperature, high-pressure, corrosive operating environment.

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

Performer: Ohio State University Research Foundation

Award Number: FE0008960

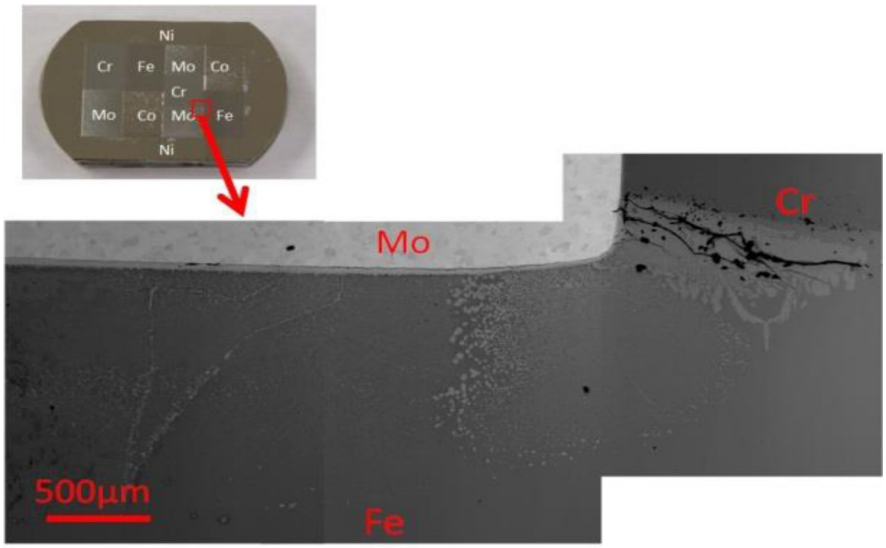
Project Duration: 9/1/2012–8/31/2015

Total Project Value: $299,934

Funding Source: 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.

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

Performer: Tennessee State University

Award Number: FE0011549

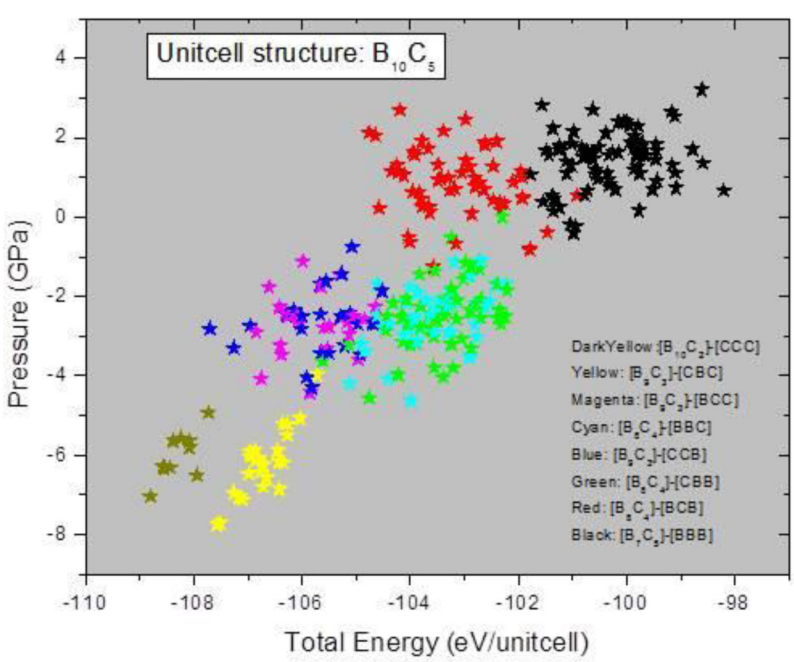
Project Duration: 9/1/2013–8/31/2015

Total Project Value: $200,000

Funding Source: 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.

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

Performer: University of Tennessee

Award Number: FE0008855

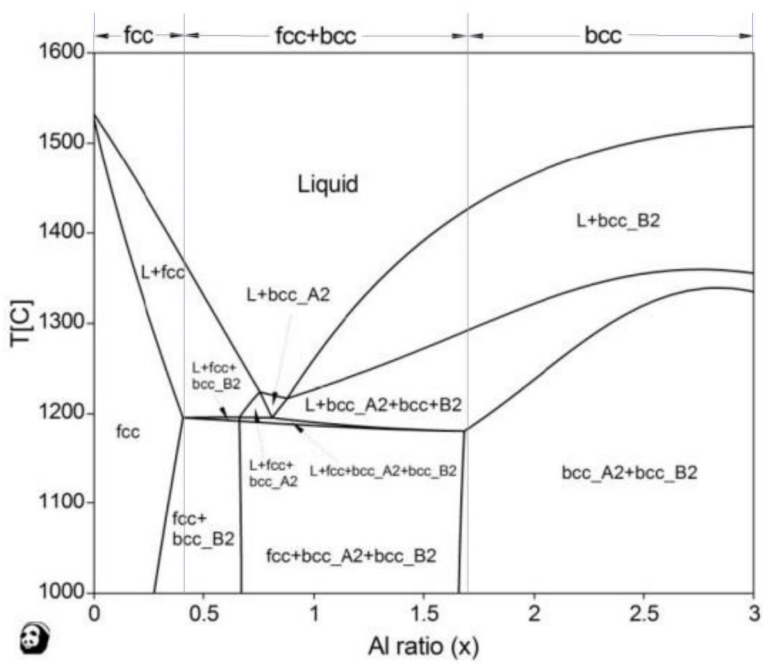
Project Duration: 8/1/2012 – 7/31/2015

Total Project Value: $300,000

Funding Source: 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 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 AlXCoCrCuFeNi HEA system using thermodynamic descriptions. Similar calculations will be performed for the AlXCrCuFeMnNi HEA system to assist in the design of HEAs suitable for use in high-temperature applications.

Abbreviations

°C ..... degrees Celsius

°F ..... degrees Fahrenheit

3-D ..... three-dimensional

AFM ..... atomic force microscope

APS ..... air plasma sprayed

AUSC ..... advanced ultrasupercritical

BCC ..... body centered cubic

CALPHAD ..... calculation of phases diagram

CLC ..... chemical looping combustion

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

CME ..... chemical and molecular engineering

CO_2 ..... carbon dioxide

CVD ..... chemical vapor deposition

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

EBC ..... environmental barrier coating

FCC ..... face centered cubic

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

FFT ..... fast Fourier transform

GB ..... grain boundaries

GB/IGF ..... grain Boundaries/intergranular films

GE ..... General Electric

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

HEA ..... high energy alloy

HPC ..... high performance computing

HVOF ..... high velocity oxy-fuel

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

K ..... kelvin

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

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

MAX ..... MAX phases, or Mn+1AXn [M = a transition metal, A = (Al), X = (C) or (N)]

MC ..... Monte Carlo

MD ..... molecular dynamics

MOCVD ..... metal organic chemical vapor deposition

MPa ..... megapascals

NETL ..... National Energy Technology Laboratory

OC ..... oxygen carriers

ODS ..... oxide dispersion strengthened

OM ..... omega method

ORNL ..... Oak Ridge National Laboratory

OSU ..... Ohio State University

PFBC ..... pressurized fluidized bed combustion

R&D ..... research and development

ReaxFF ..... reactive force field

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

SQS ..... special quasirandom structure

TBC ..... thermal barrier coating

TEM ..... transmission electron microscopy

TG-DTA ..... thermogravimetric and differential thermal analysis

TiB_2 ..... titanium diboride

TiC ..... titanium carbide

U.S. ..... United States

UCR ..... University Coal Research [NETL program]

USC ..... ultrasupercritical

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

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

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