NETL

Crosscutting Research & Analysis Program Advanced Manufacturing Project Portfolio

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U.S. DEPARTMENT OF ENERGY

the **ENERGY** lab
National Energy Technology Laboratory

Disclaimer

Contents

Introduction

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

The Crosscutting Research and Analysis 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 and Analysis Program also sponsors one of the longest running and most important university training and research programs to reinforce the research-based education of students at U.S. universities and colleges with emphasis on fossil energy science. The major objective for this program is to produce tools, techniques, and technologies that map to the Clean Coal Research Program efforts.

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

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

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

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

The Crosscutting Research and Analysis Program comprises these key technology areas:

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

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

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

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

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

Advanced Manufacturing

Advanced manufacturing is emerging as an especially potent driver of future economic growth. A distinguishing feature of advanced manufacturing is its continual improvement in processes and rapid introduction of new products. It is this paradigm-shifting aspect of advanced manufacturing that has the most potential to spin off entirely new industries and lead to production methods that are most likely to "stick" in the United States because they are hard to imitate. The Innovative Manufacturing Initiative of the Department of Energy is one element of the Federal portfolio that is seeking to accelerate advanced manufacturing process innovation. It is funding cost-shared R&D of processes that have the potential to significantly reduce energy and carbon intensity over the coming decades. By doing so, the initiative aims to revitalize existing manufacturing industries as well as support the development of emerging industries.

In 2010, the America COMPETES Reauthorization Act Section 102 directed the National Science and Technology Council (NSTC) to develop a strategic plan to guide Federal programs and activities in support of advanced manufacturing research and development. In 2011 President Obama announced establishment of the Advanced Manufacturing National Program Office (AMNPO), the Advanced Manufacturing Partnership (AMP), and the National Network for Manufacturing Innovation (NNMI).

According to the NSTC, "advanced manufacturing is a family of activities that (a) depend on the use and coordination of information, automation, computation, software, sensing, and networking, and/or (b) make use of cutting-edge materials and emerging capabilities enabled by the physical and biological sciences, for example nanotechnology, chemistry, and biology. It involves both new ways to manufacture existing products, and the manufacture of new products emerging from advanced technologies." [NSTC 2012]

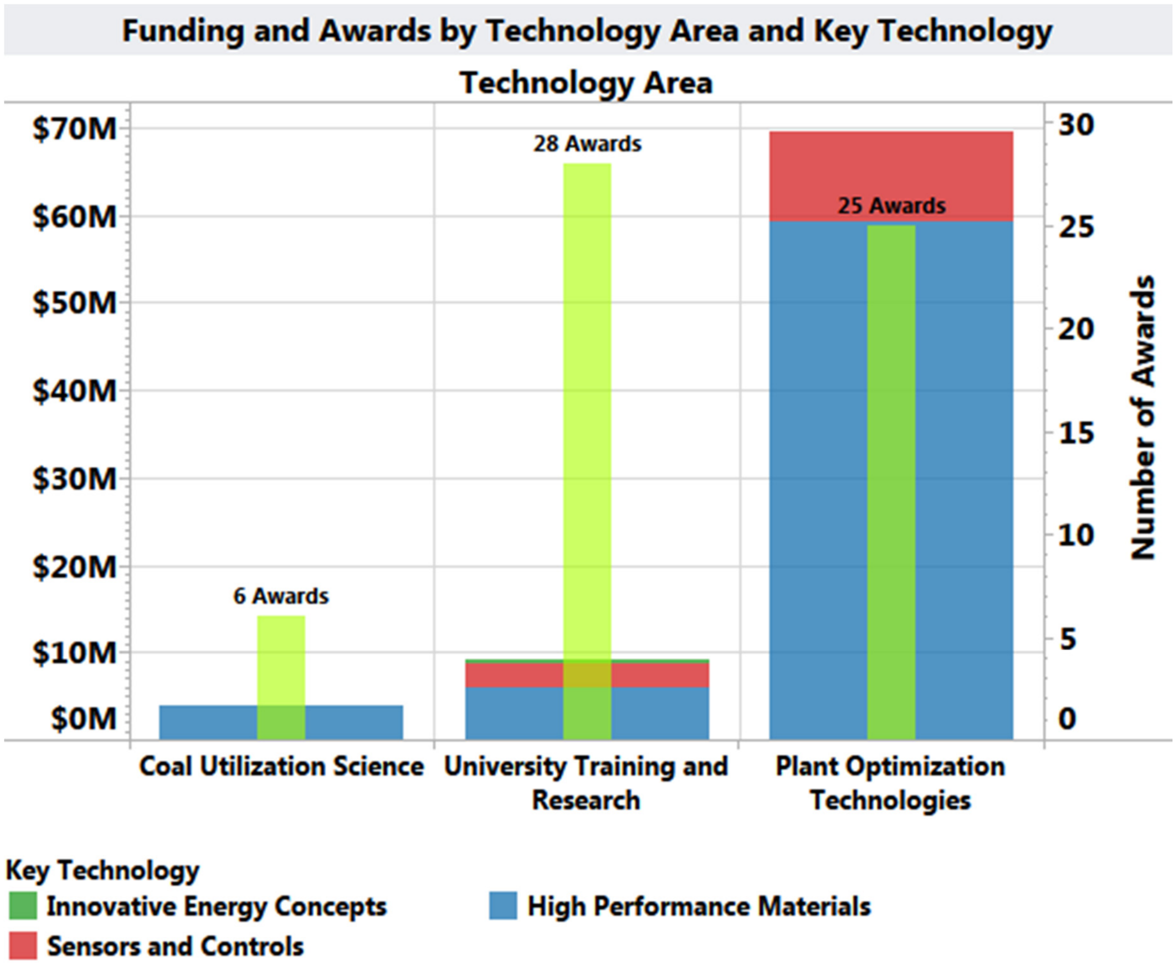
Within the Department of Energy, advanced manufacturing may also be defined in terms of improvements in lifecycle energy use. Advanced manufacturing methods and products that lead to reduced energy consumption are a focus.

NETL Programs Related to Advanced Manufacturing

As DOE's Fossil Energy technology R&D laboratory, NETL has been active in developing advanced manufacturing related technologies. These programs have been identified as sources of advanced-manufacturing technology developments:

Crosscutting Research Advanced Manufacturing Related Funding:

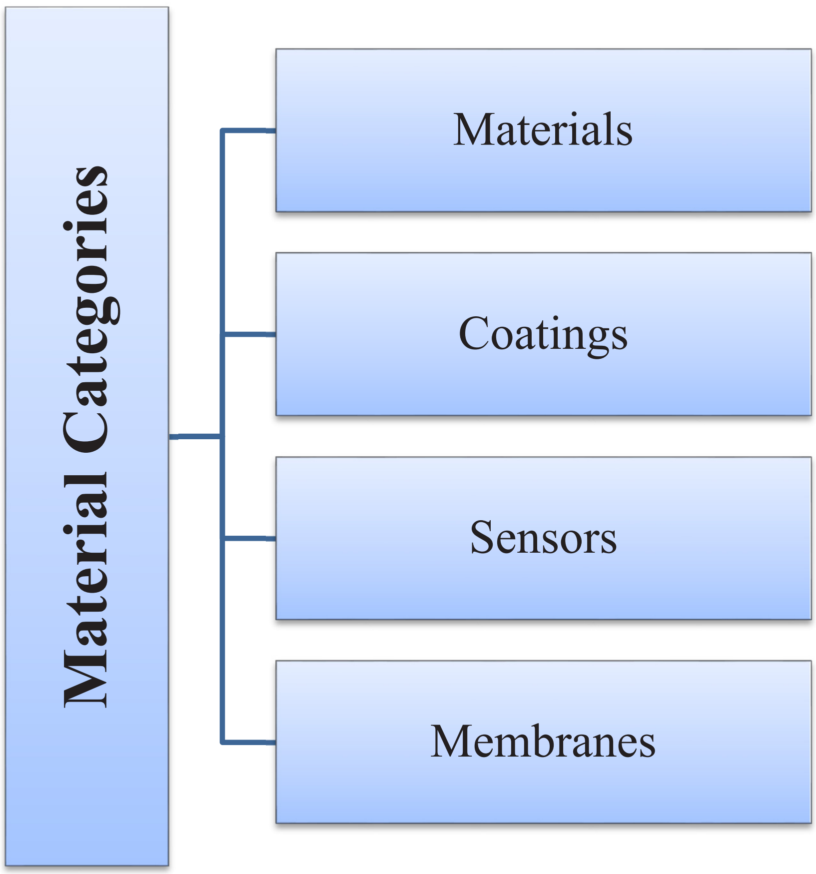
The graphic below represents Crosscutting Research Advanced Manufacturing funding and number of awards by technology area and key technology.


Funding and Awards by Technology Area and Key Technology
Technology Area
$70M
$60M
$50M
$40M
$30M
$20M
$10M
$0M
28 Awards
25 Awards
6 Awards
30
25
20
15
10
5
0
Number of Awards
Coal Utilization Science
University Training and Research
Plant Optimization Technologies
Key Technology
Innovative Energy Concepts
High Performance Materials
Sensors and Controls

Project Pages

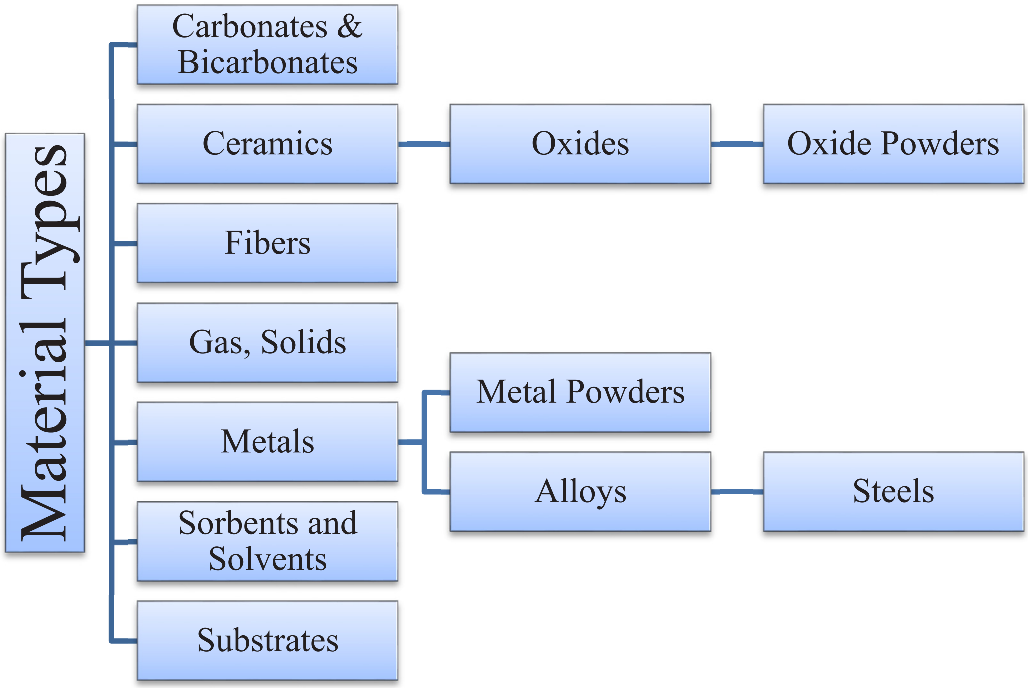
Each project identified as having relevance to advanced manufacturing is described in this report in a one-page summary. Key elements of these pages are as follows:

- ***Material Category/ Material Type***
    - **Material Category**: higher-level container for Material Type. The four broad categories used are presented graphically below.



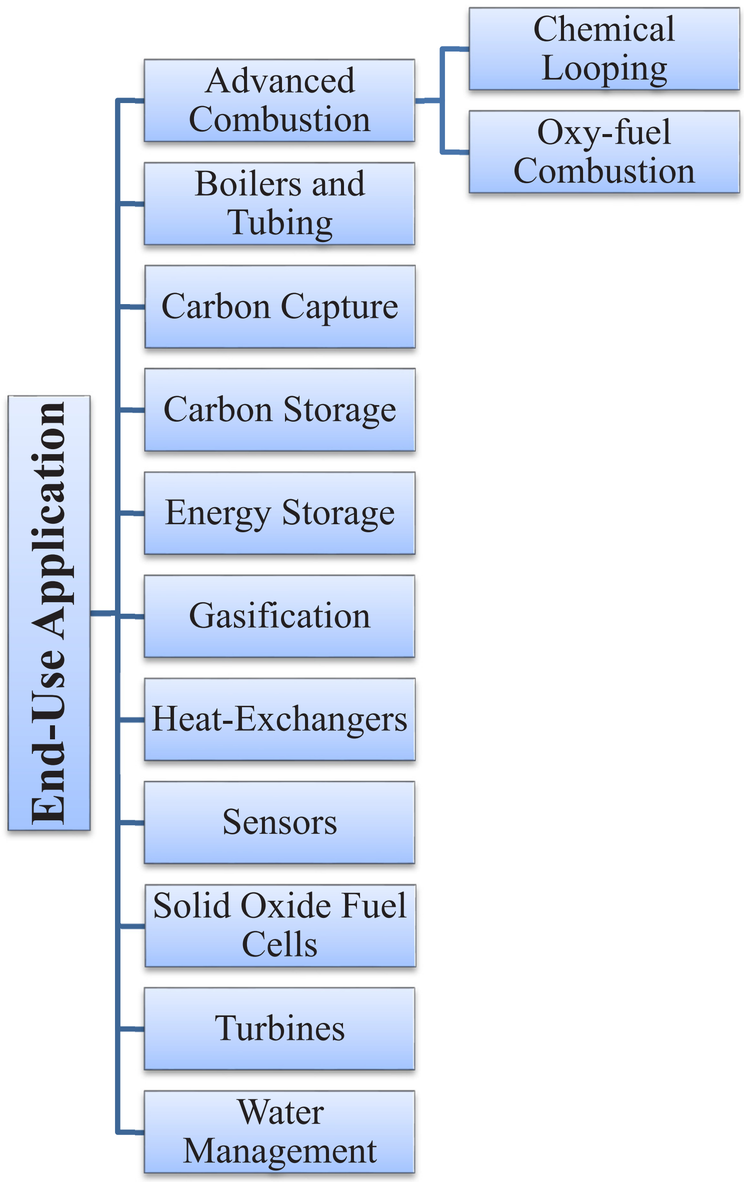
The Material Category descriptor may be substantial, as in Materials; functional, as in Sensors, or both, as in Coatings, or Membranes.

- **Material Type** (see graphic below): categorizes the nature of the material at issue substantially (e.g., Gas, Solids; Fibers; Metals) or functionally (e.g., Sorbents, Solvents). See graphic below. Where the Material Category is a functional description rather than a substance, Material Type may refer to the application (e.g., sensors used to monitor refractory materials of alloys or ceramics).

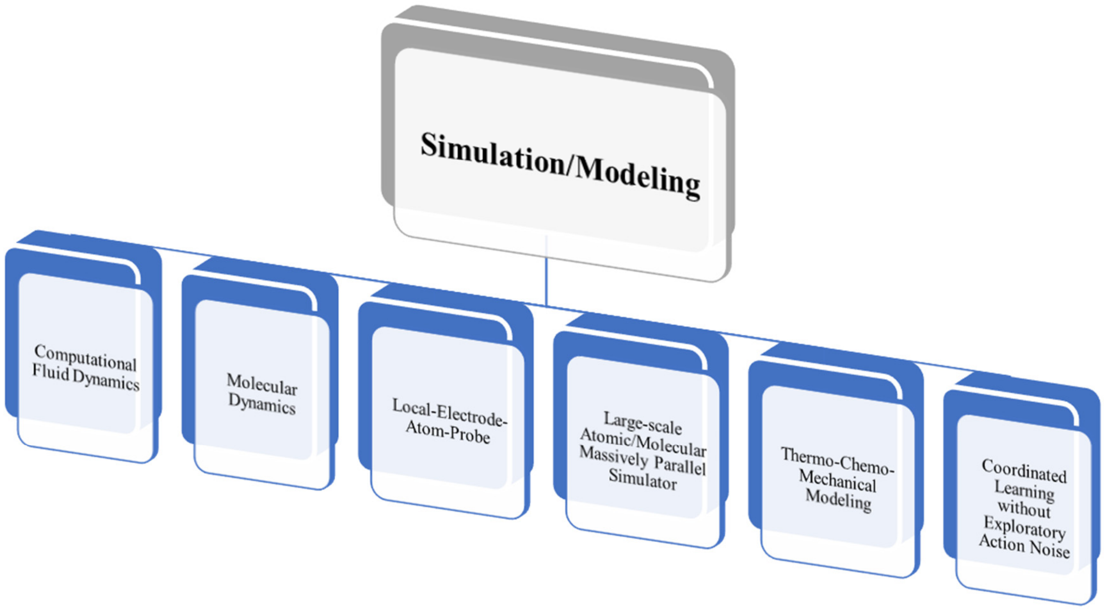


Information specifying exact materials is provided under this heading when appropriate.

- ***End-Use Application*** – The high-level end-use applications are shown below.



- **Simulation and Modeling** is a subsection of Manufacturing Systems, understood as a set of design support tools.



Color Legend

Boxes on the project pages are color coded to differentiate Computational Modeling, Additive Manufacturing/3-D Printing, and Other processes.

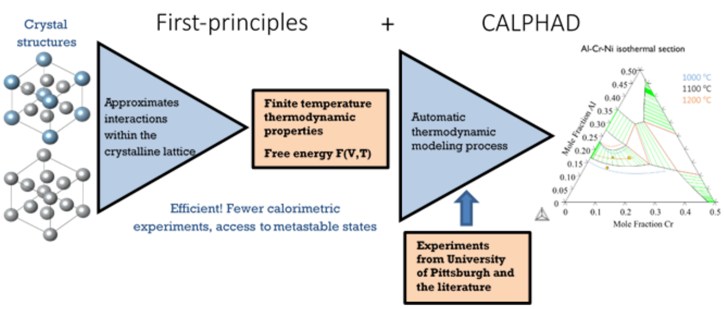
Coal Utilization Sciences

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

Performer: Pennsylvania State University
Award Number: FE0024056
Project Duration: 01/01/2015 – 12/31/2016
Total Project Value: $ 632,176
Technology Area: Coal Utilization Science
Key Technology: High Performance Materials

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

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



Materials Category/ Type
(Coatings/Alloys) Nickel-based alloys, Ni-Al-Cr-Co-Si-Hf-Y system

Manufacturing/Fabrication Process/Method
Calculation of Phase Diagram (CALPHAD) software/database, density functional theory, thermodynamic modeling

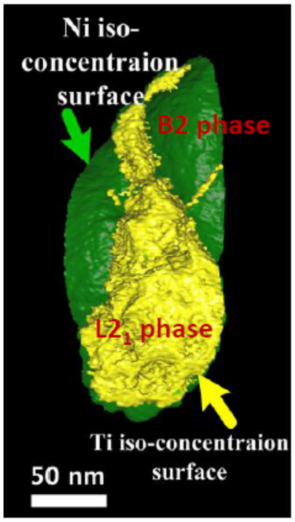
End Use:
Boilers and tubing

Computational Design and Performance Prediction of Creep-Resistant Ferritic Superalloys

Performer: University of Tennessee
Award Number: FE0024054
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 626,681
Technology Area: Coal Utilization Science
Key Technology: High Performance Materials

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

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



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

Materials Category/ Type:
Materials/Alloys
Ferritic alloys, B2/L21 particles

Manufacturing/Fabrication Process/ Method:
Computation of bulk thermodynamic properties (formation and ordering energies), interfacial energies, and elastic constants
End Use:
Steam turbines

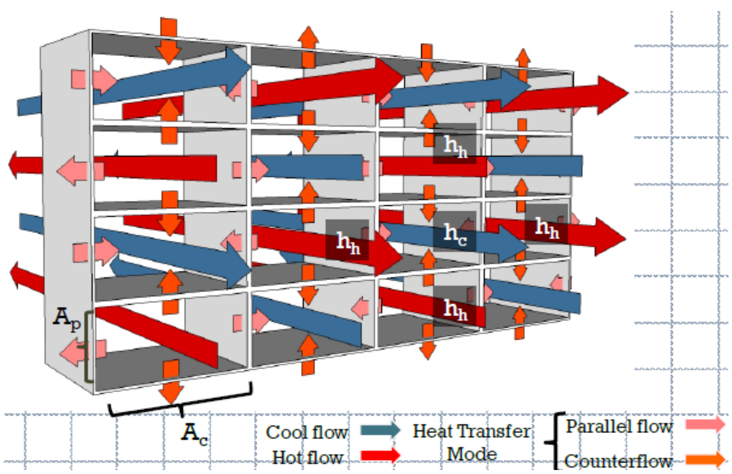
Coal Utilization Sciences

High Temperature Ceramic Heat Exchanger for Solid Oxide Fuel Cell

Performer: Mohawk Innovative Technology, Inc.
Collaborator(s): FuelCell Energy
Award Number: FE0024090
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 643,682
Technology Area: Coal Utilization Science
Key Technology: High Performance Materials

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

This project will lead to the development of an advanced manufacturing technique for ceramic materials.



Recuperator Geometry.

Materials Category/ Type
Materials, Coatings/Alloys, Ceramics, Metals: Silicon carbide, silicon nitride, alumina-based materials, hybrid cermet materials

Manufacturing/Fabrication Process/Method
Brazing, bonding, and joining

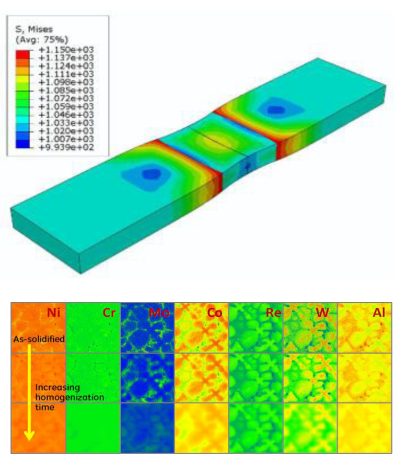
End Use:
SOFC, Gas turbine recuperator, Heat exchanger

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

Performer: General Electric Company
Award Number: FE0024027
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 649,707
Technology Area: Coal Utilization Science
Key Technology: High Performance Materials

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

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



Multi-component and multiphase diffusion modeling3D Model.

Materials Category/ Type
Materials/Alloys
Haynes 282

Manufacturing/Fabrication Process/Method
Finite element modeling; microstructure and crystal plasticity (CP) models; constitutive creep modeling

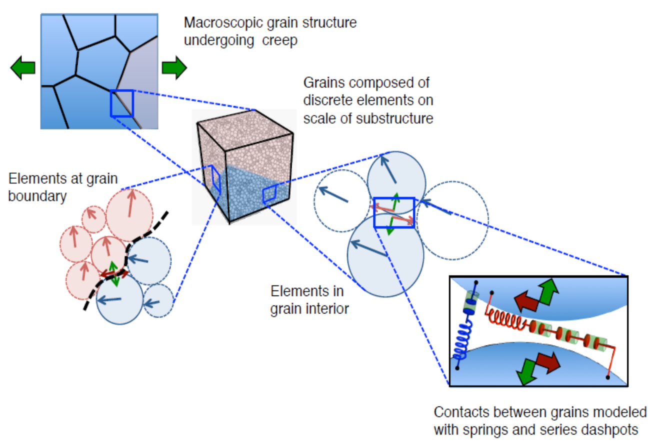
End Use: Boilers and tubing, gas turbine combustor

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

Performer: Oregon State University
Award Number: FE0024065
Project Duration: 01/01/2015 – 12/31/2016
Total Project Value: $ 624,999
Technology Area: Coal Utilization Science
Key Technology: High Performance Materials

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

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



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

Materials Category/ Type
Materials/Alloys
Nickel-based alloy

Manufacturing/Fabrication Process/Method
Discrete element method (DEM); molecular dynamics, kinetic Monte Carlo modeling

End Use:
Boiler, turbine

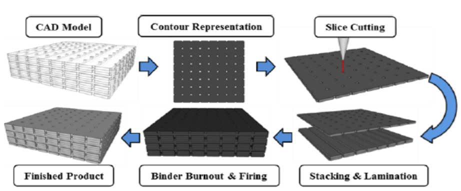
Plant Optimization Technologies

Siemens Corporation	Novel Temperature Sensors and Wireless Telemetry for Active Condition Monitoring of Advanced Gas Turbines	43
West Virginia University Research Corporation	Smart Refractory Sensor Systems for Wireless Monitoring of Temperature Health and Degradation of Slagging Gasifiers	44
Pacific Northwest National Laboratory	Solid State Joining of Creep Enhanced Ferritic Steels	45
Energy Industries of Ohio, Inc.	Steam Turbine Materials for Advanced Ultra Supercritical (AUSC) Coal Power Plants	46
Oak Ridge National Laboratory	Ultra-Supercritical Steam Cycle Turbine Materials	47
Oak Ridge National Laboratory	Weldability of Creep Resistant Alloys for Advanced Power Plants	48

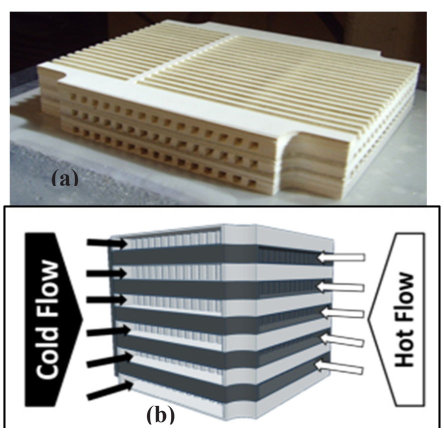
Additive Manufacturing for Cost Efficient Production of Compact Ceramic Heat Exchangers and Recuperators

Performer: Ceralink Inc.
Award Number: FE0024066
Project Duration: 11/01/2014 – 10/31/2015
Total Project Value: $ 639,345
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

NETL partnered with Ceralink Inc. to use additive manufacturing (AM) for the design and build of a prototype high-temperature and compact ceramic heat exchanger as a key component for high efficiency advanced power generation systems. An AM technique, known as laminated object manufacturing (LOM), uses precision laser cutting of ceramic green tapes, which are then stacked to build a 3D object with fine internal features. Modeling was used to develop prototype designs and predict efficiency in the ceramic heat exchangers. During the development process, new LOM protocols were established including laser optimization, strategies for fine feature integrity, lamination fluid control, green handling, and firing. Three full-size prototypes were fabricated using two different designs. Performance testing showed the prototypes could successfully withstand the high temperature operating conditions, but further work is needed to verify the anticipated 25% increase in system level recuperator thermal efficiency. A weight to volume ratio greater than 50% compared to metal heat exchangers is an important benefit of using ceramic recuperators. The benefits of thermal efficiency and weight reductions have a significant impact on energy savings in aerospace and distributed combined heat and power generation, and provide reductions in CO_2, NOX, and SOX emissions.



LOM builds 3D parts from 2D ceramic



a) Prototype – cut illustration channel, b) Model of a scale-up generation 1 part

Materials Category/ Type
Materials/Ceramic
Aluminum nitride, zirconium dioxide

Manufacturing/Fabrication Process/Method
Laminated Object Manufacturing (LOM); Microwave assist technology (MAT™)

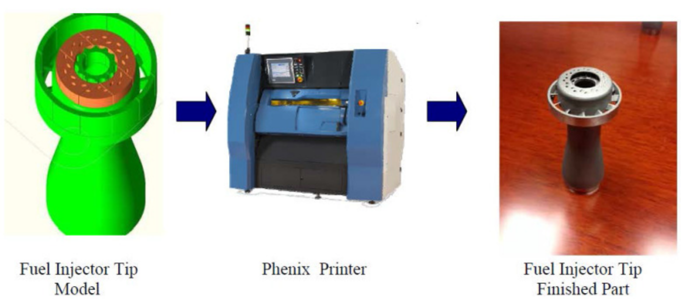
End Use:
Heat exchangers

Additive Manufacturing of Fuel Injectors

Performer: Edison Welding Institute, Inc.
Award Number: FE0023974
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 622,384
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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



50,000 foot view of AM Courtesy of EWI.

Materials Category/ Type
Alloys/Metal Powders
Nickel-based alloys; Hastelloy / Alloy X

Manufacturing/Fabrication Process/Method
Additive manufacturing (AM) technique, Laser powder bed fusion (L-PBF), Abrasive flow machining

End Use:
Turbines

Additive Manufacture of Smart Parts with Embedded Sensors for In-Situ Monitoring in Advanced Energy Systems

Performer: Missouri University of Science and Technology
Award Number: FE0012272
Project Duration: 10/01/2013 – 09/30/2016
Total Project Value: $1,879,427
Technology Area: Plant Optimization Technologies
Key Technology: Sensors and Controls

The main objective of this three-year program is to conduct fundamental and applied research that will lead to successful development and demonstration of "smart parts" with embedded sensors for in-situ monitoring of multiple parameters. Such measurements are imperative to the realization of safe operation and optimal control of advanced energy systems for enhanced reliability, improved efficiency and reduced emission.

The proposed research focuses on solving the fundamental and engineering challenges involved in design, fabrication, integration, and application of the proposed novel "smart liner block" and "smart pipes". Innovative research will be conducted in the following subjects: (a) robust, embeddable optical carrier-based microwave interferometry (OCMI) sensors for in-situ measurement of temperature (up to 1600 degrees Celsius), pressure and refractory wall cracking and thinning; (b) novel signal processing and instrumentation for distributed sensing; (c) comprehensive thermal and mechanical models of the sensor-integrated "smart parts" for optimal sensor embedment and rational interpretation of the sensor outputs; (d) multifunctional protective layers between OCMI sensor and the host materials for thermal, mechanical and chemical protection of the sensors; and (e) additive manufacturing of the smart parts with embedded sensors

The research will be carried out in two phases. Phase I will focus on the proof of the smart part concept through the development and characterization of the individual components including the OMCI sensors, instrumentation, thermal and mechanical models, protective layers and additive manufacturing techniques/processes. In Phase II, these components will be integrated and optimized to construct smart blocks and pipes for systematic technology evaluation and demonstration under simulated conditions using test facilities in the laboratory.

Dual-laser additive manufacturing (AM) system for fabrication of "smart parts".

Materials Category/ Type
Sensors/Ceramics

Manufacturing/Fabrication Process/Method
Additive manufacturing; freeze-form extrusion fabrication (FEF)

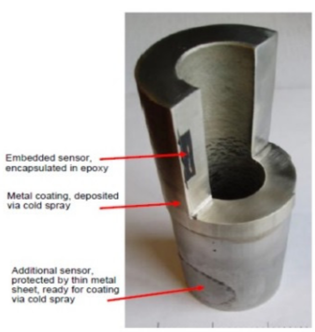
End Use:
Sensors, Turbines, Embedded sensors in airfoils of industrial gas turbines

Additive Topology Optimized Manufacturing with Embedded Sensing

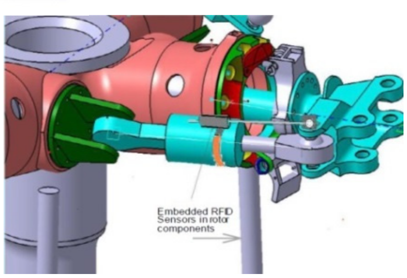
Performer: United Technologies Corporation Research Center
Award Number: FE0012299
Project Duration: 10/01/2013 – 09/30/2016
Total Project Value: $1,482,700
Technology Area: Plant Optimization Technologies
Key Technology: Sensors and Controls

United Technologies Research Center (UTRC) will seamlessly embed a suite of sensors into the industrial gas turbine airfoil to demonstrate additive manufacturing as a relevant process (when guided by physics-based models) for next-generation gas turbines. The resulting "smart part" will: be remotely powered and sensed, maintain its structural integrity, and provide real-time diagnostics when coupled to a Health-Utilization-Monitoring System (HUMS)

UTRC will use physics-based models to predict the impact of placing the sensing element into a highly demanding structural component such as an INGT airfoil. The structural and process models will be used to minimize structural impact, while positioning the sensor suite for maximum information content subject to the structural constraint. Electromagnetic modeling will be used to concomitantly predict transfer of radio frequency power and signal level as a result of embedding the sensors in a metal housing. A cold spray process will be used to actually embed the sensors into the airfoil, followed by extensive structural and electromagnetic testing. Finally, a wireless communication transponder and high-bandwidth uplink will be used to demonstrate real-time data analysis of the sensor suite using a health and utilization monitoring system.



Embedded sensor locations.



Materials Category/ Type
Sensors/ Alloys

Manufacturing/Fabrication Process/Method
Additive manufacturing; Additive Topology Optimized Manufacturing with Embedded Sensing (ATOMeS) process methodology; high-velocity metal powder cold spray deposition; direct metal laser sintering (DMLS)

End Use: Sensors, Turbines, Embedded sensors in airfoils of industrial gas turbines

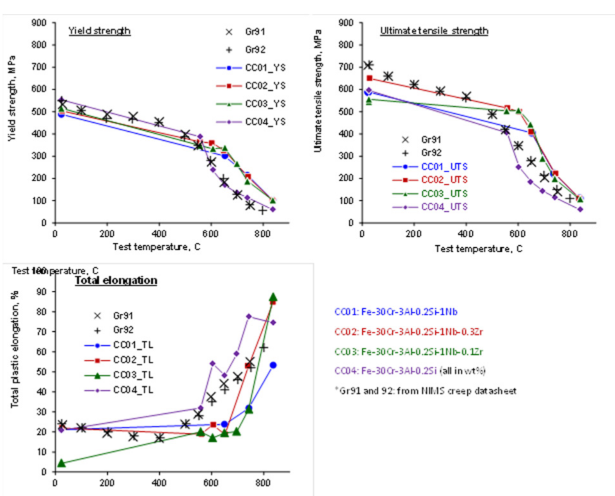
Advanced Alloy Design Concepts for High Temperature Fossil Energy Applications

Performer: Oak Ridge National Laboratory
Award Number: FWP-FEAA114
Project Duration: 10/01/2013 – 09/30/2016
Total Project Value: $1,034,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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

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



Tensile Properties of New High Temperature Alloys.

Materials Category/ Type
Materials/Alloys, Steels
FeCrAl Alloys, Cr-Ferritic-Martensitic Steels, Austenitic Steels, Ni-Based Alloys, T91, Inconel 740

Manufacturing/Fabrication Process/Method
Inter-diffusion and thermodynamic modeling

End Use: Boilers and tubing, heat-exchanger tubes

Plant Optimization Technologies

Advanced Ceramic Materials and Packing Technologies for Realizing Sensors Operable in Advanced Energy Generation Systems

Performers: Sporian Microsystems, Inc.
Collaborator(s): Honeywell, Pratt & Whitney, Boeing, Rolls-Royce, Siemens, Lockheed Martin, NavAir, Williams International, Ohio Aerospace Institute, and Propulsion Instrumentation Working Group
Award Number: SC0008269
Project Duration: 06/28/12 – 08/13/2015
Total Project Value: $2,159,500
Technology Area: Plant Optimization Technologies
Key Technology: Sensors and Controls

This novel concept attempts to develop ultra-high temperature "smart" sensors from silicon carbon nitride (SiCN) materials for energy generation and aerospace systems. The sensors will be developed from innovative fabrication processes and contain internal compensation, health check and data bus support to the interface.

In order to do this, the project will build a sensor utilizing a class of high-temperature ceramic materials synthesized by thermal decomposition of polymeric precursors, which possess excellent mechanical properties up to 1800°C. Secondly, the team will construct and fabricate designs for multiple sensors to produce bench- and pilot-scale operable demonstration-ready sensing.

By continuous condition monitoring of high temperature surrounding using these sensors, one can expect to lower failure rates, improved contact and reduced moisture collection with sensing at the source and an overall lower cost associated with life and system failures.

Materials Category/ Type
Materials/Ceramics (SiCN)

Manufacturing/Fabrication Process/Method
Thermal decomposition

End Use
Integrated Gasification Combined Cycle (IGCC); Natural Gas Combined Cycle (NGCC)

Advanced Ultrasupercritical (AUSC) Tube Membrane Panel Development

Performer: Alstom Power, Inc
Award Number: FE0024076
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 666,667
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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

Straight flat panels in shop.

Boiler wall layout in shop.

Materials Category/ Type
Materials/Coatings, Alloys
T91, T92, HR6W, VM12, ferritic, austenitic, and nickel-based alloys

Manufacturing/Fabrication Process/Method
Undisclosed

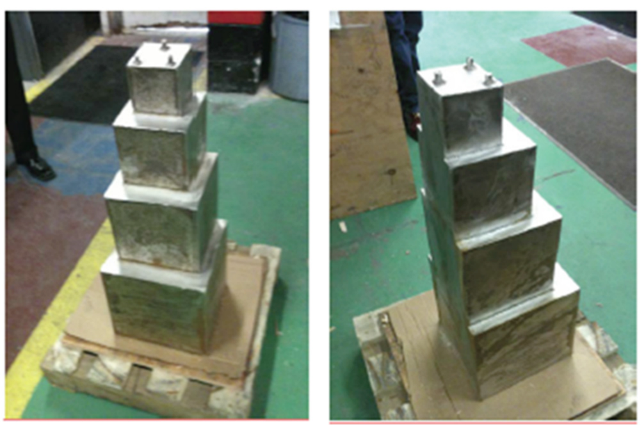
End Use:
Boilers, Power plants

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

Performer: Energy Industries of Ohio Inc.
Award Number: FE0024014
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 625,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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



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

Materials Category/ Type
Materials/Alloys, Powders, Haynes Alloy A-282 metal, 316L Stainless Steel

Manufacturing/Fabrication Process/Method
Additive manufacturing, 3D Printing, HIP

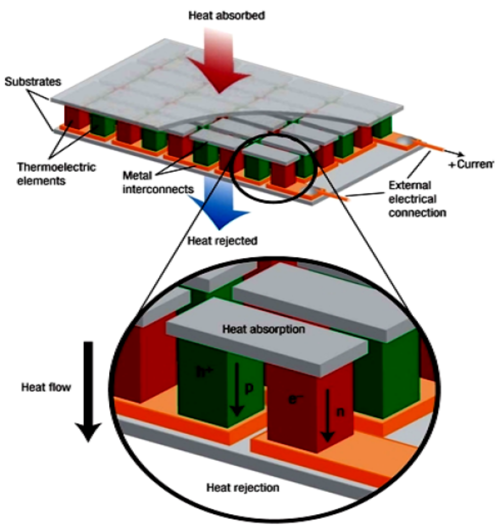
End Use:
Boilers, Turbines

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

Performer: West Virginia University Research Corporation
Award Number: FE0024009
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 627,160
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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



Thermoelectric Module

Materials Category/ Type
Materials/Oxide Powders
$CaMnO_3$, $Ca_3Co_4O_9$, SiO_2

Manufacturing/Fabrication Process/Method
Tape casting, chemical sol-gel process

End Use:
Thermoelectric generators, Heat recuperators, Waste heat recovery from turbines, SOFCs, Ceramic heat exchangers

Plant Optimization Technologies

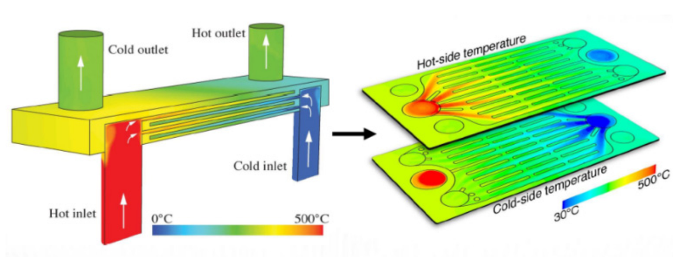
Plant Optimization Technologies

Compact, Ceramic Microchannel Heat Exchangers

Performer: Ceramatec, Inc.
Award Number: FE0024077
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 499,922
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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



Heat exchanger plate design and analysis.

Materials Category/ Type
Materials/Alloys/Ceramics, Plates

Manufacturing/Fabrication Process/Method
Laminated object manufacturing (LOM); computational modeling using ASPEN, FLUENT; brazing, glass seals, mechanical seals, diffusion bonding.

End Use:
Heat Exchangers, SOFC, Microturbine

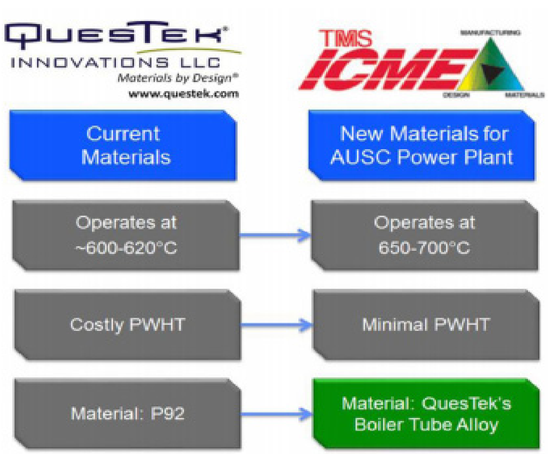
Computational Design of Weldable, High-Cr Ferritic Steel

Performer: QuesTek Innovations LLC
Award Number: SC0006222
Project Duration: 06/18/2011 – 08/07/2016
Total Project Value: $ 1,149,906
Technology Area: Plant Optimization Technologies

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

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

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



Materials Category/ Type
Materials/Alloys

Manufacturing/Fabrication Process/Method
Computational Modeling

End Use: Boilers and Tubing
Ultrasupercritical Boiler Tubes

Development of Advanced Materials for Ultrasupercritical Boiler Systems

Performer: Energy Industries of Ohio Inc.
Collaborator(s): Riley Power Inc. (formally Riley Stoker Corp.), Oak Ridge National Laboratory – ORNL, McDermott Technology Inc., ALSTOM Power Inc. - US Power Plant Laboratories, Foster Wheeler Development Corporation, Babcock and Wilcox Corporation., Electric Power Research Institute - EPRI
Award Number: FG26-NT41175
Project Duration: 10/01/2001 – 09/30/2015
Total Project Value: $33,179,639
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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

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

Corrosion due to steamside oxidation.

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

Materials Category/ Type
Materials/Alloys

Manufacturing/Fabrication Process/Method
CFD Modeling, Weld Overlay Cladding, Recrystallization

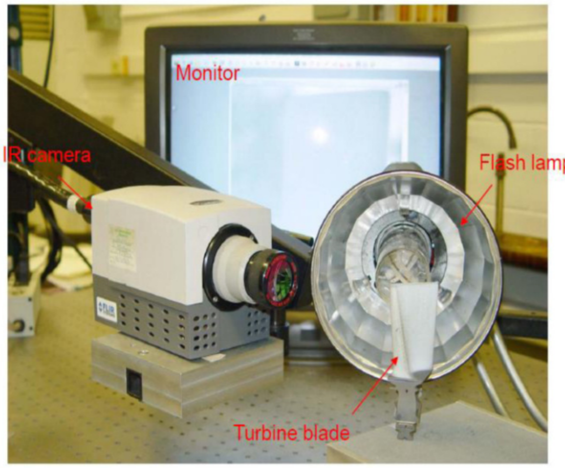
End Use: Boilers and tubing; ultra-supercritical boiler tubes

Development of Nondestructive Evaluation (NDE) Methods For Structural and Functional Materials

Performer: Argonne National Laboratory (ANL)
Collaborator(s): Siemens
Award Number: FWP-49943
Project Duration: 10/01/2013 – 09/30/2016
Total Project Value: $394,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

NETL is partnering with Argonne National Laboratory on this project. The non-destructive evaluation (NDE) development is currently focused on thermal barrier coatings 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 thermal barrier coatings (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.

Materials Category/ Type
Materials, Coatings, Membranes/Ceramics

Manufacturing/Fabrication Process/Method
Nondestructive evaluation, , infrared thermal imaging, X-ray radiation imaging, electron beam physical vapor deposition, air-plasma spraying

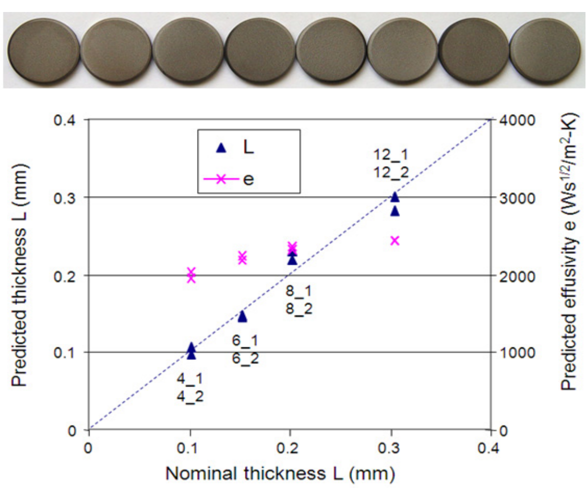
End Use
Boilers and tubing, Turbines, Membranes, Solid oxide fuel cells, Coatings

Gas Turbine Materials Life Assessment and Non-Destructive Evaluation

Performer: Argonne National Laboratory (ANL)
Collaborator(s): Siemens Corporation
Award Number: FWP-49022
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $ 910,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

This work will allow for development and improvement of advanced materials technologies and may lead to maximization of power plant efficiencies while minimizing CO_2 emissions.



Flash thermography for metallic coatings.

Materials Category/ Type
Materials/Coatings
Alloys: IN939, CM247, Rene80, X45, ECY768 and IN738

Manufacturing/Fabrication Process/Method
Nondestructive evaluation method; flash thermography

End Use:
Gas Turbines

High-Temperature Sapphire Pressure Sensors for Harsh Environments

Performer: University of Florida
Collaborator(s): Florida State University
Award Number: FE0012370
Project Duration: 01/01/2014 – 12/31/2016
Total Project Value: $1,098,191
Program/Technology Area: Plant Optimization Technologies
Key Technology: Sensors and Controls

The University of Florida, in collaboration with Florida State University, began work focused on the development of sapphire manufacturing technologies for high-temperature sensor fabrication and packaging by combining ultra-short pulse laser micromachining (LM) and spark plasma sintering (SPS). Specifically, the primary objective of this project is to develop sensor materials and designs to achieve the manufacture of sensors that enable physical parameters to be measured in situ and on line under extreme conditions such as high temperature and pressure and corrosive environments.

The proposed research will implement a multi-faceted approach to develop and quantify manufacturing technologies for the fabrication of sapphire high-temperature sensors. Laser micromachining processes will be developed using an Oxford Laser J-355PS Picosecond Laser Micromachining Workstation. SPS will be used to develop processes for joining sapphire and alumina substrates. These two technologies will enable the creation of three-dimensional microscale sapphire structures by bonding planar laser micromachined substrates via SPS. Performance of the machined components will be simulated and experimentally quantified via fracture and dislocation mechanics methods.

These technologies will enable the manufacture of miniature sapphire sensors for a variety of applications of interest such as pressure, temperature, stress/strain, etc., although for the purposes of this proposal the primary application will be an optical pressure sensor capable of operation in environments in excess of 1000 °C and pressures up to 1000 psi. The proposed research is applied in nature and will result in the establishment of critical functions regarding LM and SPS materials synthesis as well as a packaged and experimentally characterized pressure sensor

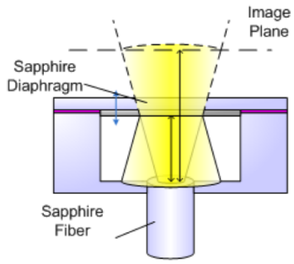
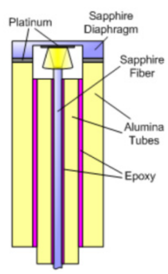


Illustration of the fiber-optic lever transduction scheme implemented in the pressure sensor design.



Schematic of sensor and packaging for the high-temperature pressure sensor.

Materials Category/ Type
Sensors/Sapphire, alumina, platinum

Manufacturing/Fabrication Process/Method
Thermocompression bonding, picosecond laser micromachining, spark plasma sintering (SPS)

End Use: Sensors

Plant Optimization Technologies

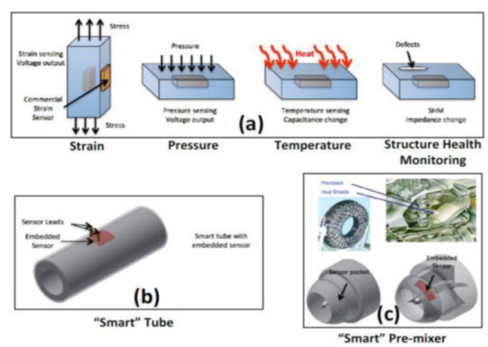
Investigation of Smart Parts with Embedded Sensors for Energy System Applications

Performer: University of Texas at El Paso
Award Number: FE0012321
Project Duration: 10/01/2013 – 09/30/2016
Total Project Value: $1,150,894
Technology Area: Plant Optimization Technologies
Key Technology: Sensors and Controls

A need for laboratory-scale experiments for fabrication, testing, and characterization of smart parts and their relevance to fossil energy systems has been established. This work proposes to develop smart parts with embedded strain, pressure, temperature, and structural health monitoring sensors. A high-Curie-temperature piezoceramic and titanium will be used to fabricate the smart parts and they will be tested in three case studies simulating realistic energy system components. Expected deliverables include design, fabrication, and characterization of the smart parts, validation of the sensing capabilities, and documentation of the sensor performance in a harsh energy system environment.

This research project aims to optimize advanced three-dimensional manufacturing processes for embedded sensors in energy system components, characterize the performance and properties of these smart parts, and assess the feasibility of applying these parts in harsh energy system environments. Specific project objectives are to (1) fabricate energy system related components with embedded sensors, (2) evaluate the mechanical properties and sensing functionalities of the smart parts with embedded piezoceramic sensors, and (3) assess the in-situ sensing capability of such energy system parts. This research effort will not only contribute to designing and fabricating parts, but also to determining the smart part's durability, repeatability, and stability by testing them in realistic energy environs.

This project aims to develop advanced technologies to 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



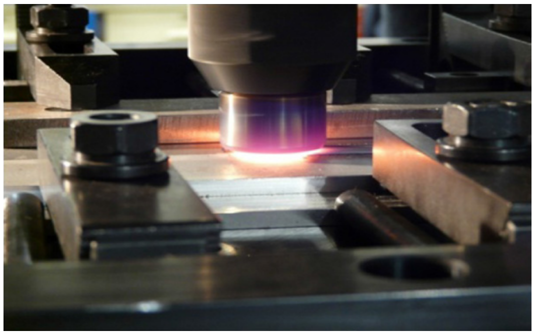
"Smart Parts" with embedded sensors, (a) sensing capabilities showcase, (b) Case Study 1, "smart" tube, (c) Case Study 2, "smart" pre-mixer.

Joining of Advanced High-Temperature Materials

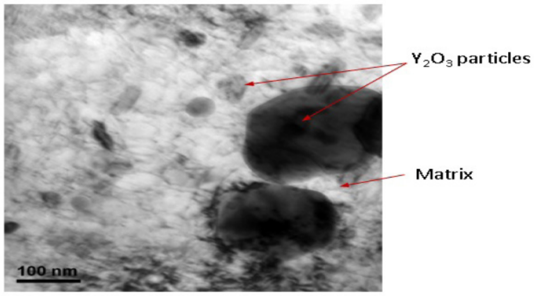
Performer: Pacific Northwest National Laboratory (PNNL)
Award Number: FWP-12461
Project Duration: 10/01/1996 – 09/30/2016
Total Project Value: $ 8,265,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

NETL is partnering with PNNL to develop a joining technology (advanced high-temperature materials) required for high-efficiency, low-emissions fossil energy conversion. PNNL will focus on ODS alloys and nickel-based superalloys. Improvement to high-temperature advanced-materials will promote the development of designs for advanced power plants capable of operating at higher temperatures and pressures, leading to improvements in efficiency and operational flexibility and resulting in lower capital and operating costs.

This project will prove that friction stir welding can be used to fuse materials that can withstand the environment within an ultrasupercritical boiler to enable cost-effective oxy-combustion systems through creep testing, microstructure characterization, and mechanical properties testing.



Friction stir welding of ¼" thick dispersion strengthened Sandivik APMT plate.



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

Materials Category/ Type
Materials/Alloys, Steels
Creep Strength Enhanced Ferritic Steels, Gr91, Gr92, Gr122, P91, P92, P122, Boron/cobalt enriched 9Cr ferritic steel

Manufacturing/Fabrication Process/Method
Solid state joining, friction stir welding

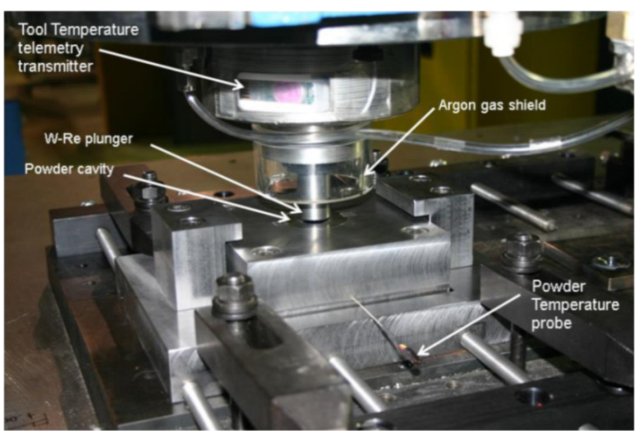
End Use: Boilers and tubing, Turbines

Low Cost Fabrication of ODS Materials

Performer: Pacific Northwest National Laboratory (PNNL)
Award Number: FWP-60098
Project Duration: 10/01/2010 – 09/30/2016
Total Project Value: $790,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

The objective of this project is to develop a low-cost method for producing high-strength, creep resistant ODS ferritic steel mill product for high-temperature applications. This project will contribute to more efficient use of fossil fuels in AUSC power plants, which will concurrently lead to reduced discharge of carbon dioxide and other emissions.



Friction Extrusion Die at Pacific Northwest National Laboratory.

Materials Category/ Type
Materials/Alloys, Steels
Oxide dispersion strengthened (ODS) alloys

Manufacturing/Fabrication Process/Method
Shear consolidation process, high-energy mechanical milling, powder metallurgy processing, hot-isostatic pressing, friction stir welding

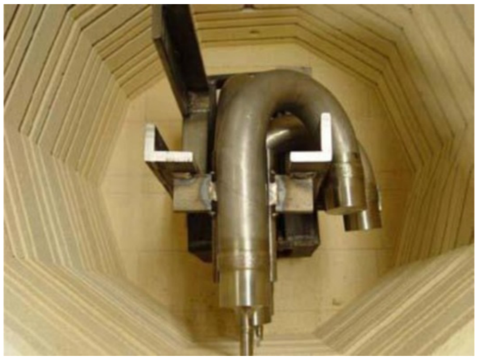
End Use: Boilers and tubing, Gasification

Materials for Ultra-Supercritical (USC) Steam Power Plants

Performer: Oak Ridge National Laboratory - ORNL
Award Number: FWP-FEAA061
Project Duration: 09/29/2009 – 09/30/2016
Total Project Value: $2,329,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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



Alloy 617 in Cold Bend Test Rig.

Materials Category/ Type
Materials/Alloys
Inconel 740, Alloy 617, Haynes 282

Manufacturing/Fabrication Process/Method
Casting, Thermodynamic modeling, Welding

End Use: Boilers and tubing, turbines

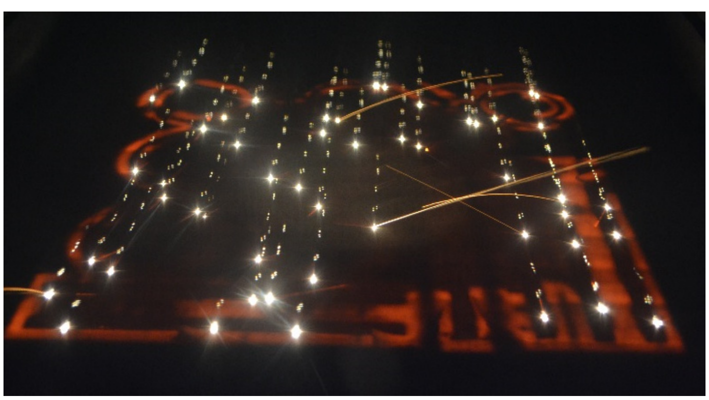
Plant Optimization Technologies

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

Performer: Oak Ridge National Laboratory - ORNL
Collaborator(s):
Award Number: FWP-FEAA119
Project Duration: 10/01/2015 – 09/30/2016
Total Project Value: $ 424,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

The technology developed is anticipated to be used to produce high-temperature gas turbine components as well as similar-size components for other advanced fossil energy applications.



Metallic part fabrication using the electron-beam melting process

Materials Category/ Type
Metals - high temperature Ni-based Hastelloy X (HX) alloy

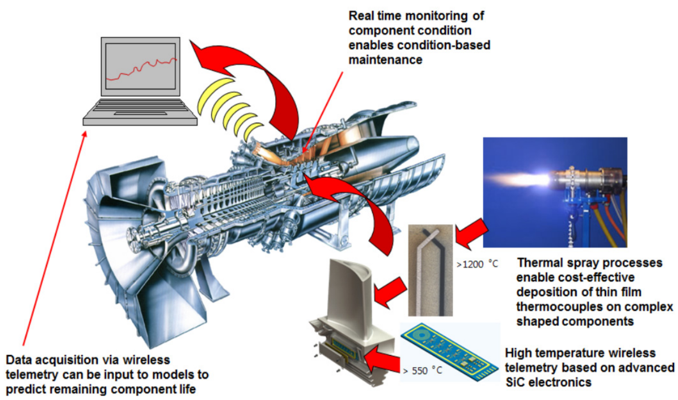
Manufacturing/Fabrication Process/Method
Additive manufacturing (AM) fabrication process - electron beam melting (EBM) at ORNL, laser metal deposition (LMD) at Siemens and selective laser melting (SLM)

End Use
Turbines

Novel Temperature Sensors and Wireless Telemetry for Active Condition Monitoring of Advanced Gas Turbines

Performer: Siemens Corporation
Collaborator(s):
Award Number: FE0026348
Project Duration: 09/16/2015 - 02/28/2017
Total Project Value: $ 937,500
Technology Area: Plant Optimization Technologies
Key Technology: Sensors and Controls

The objective of the program is to integrate durable, non-intrusive, ultra-high-temperature thermocouples (> 1200 °C) with high temperature wireless telemetry to enable materials prognostics and active condition monitoring in the hot gas path (HGP) of industrial gas turbines. The specific objectives are (1) to fabricate and install Smart Turbine Blades with thermally sprayed sensors and high temperature wireless telemetry systems in an H-Class engine, (2) to integrate the component engine test data with remaining useful life (RUL) models and develop an approach for networking the component RUL data with Siemens' Power Diagnostics engine monitoring system. Phase 1 involves scaling up the thermal spray process to develop high temperature ceramic thermocouples, development of wireless telemetry system components, and demonstration of integrated sensor/wireless telemetry approach on stationary lab test rig.



The Smart Turbine Component, consisting of integrated embedded sensors with wireless telemetry, operational in the harsh environments of the gas turbine

Materials Category/ Type
Materials/Ceramics.

Manufacturing/Fabrication Process/Method
Thermal Spray Process

End Use

Sensors, Turbines

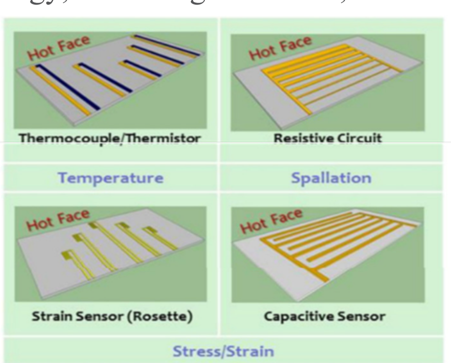
Smart Refractory Sensor Systems for Wireless Monitoring of Temperature Health and Degradation of Slagging Gasifiers

Performer: West Virginia University Research Corporation
Collaborators: ANH Refractories Company (ANH)
Award Number: FE0012383
Project Duration: 10/01/2013 – 09/30/2016
Total Project Value: $1,617,113
Technology Area: Plant Optimization Technologies
Key Technology: Sensors and Controls

The United States Department of Energy (DOE) National Energy Technology Laboratory (NETL) has partnered with West Virginia University (WVU) to develop in situ and online sensing capability for advanced energy systems operating at high temperature and pressure, in the harsh environments of advanced power generation systems. Researchers at WVU, in collaboration with ANH Refractories Company (ANH), will demonstrate a high-temperature sensor concept for monitoring reaction conditions and health within slagging coal gasifiers. The technology will include the development of smart refractory gasifier brick. The new sensors will monitor the status of equipment, materials degradation, and process conditions that impact the overall health of a refractory lining in the high-temperature, highly corrosive environments of coal gasifiers.

The key aspect of the proposed technology is that these sensors will be incorporated and interconnected throughout the volume of the refractory brick and will not negatively impact the intrinsic properties of the refractory, thereby circumventing the need to insert a sensor into the refractory via an access port. This will ensure the integrity of the sensor within the harsh environment and will not introduce flaws or slag penetration pathways within the refractory, as is typically the issue with inserting sensors through access ports.

The anticipated benefit of this project would be the development of a more reliable and non-intrusive method of monitoring gasifier temperature and refractory health than is possible with current methods. Such improvements are expected to result in lower operating and maintenance costs of slagging gasifiers. The development of the proposed smart refractory and refractory sensor system concept could be applied to other applications, such as conventional coal-fired boiler technology, biomass gasification, and steel and glass manufacturing.



Schematics depicting possible embedded sensor designs
Source: West Virginia University Project Narratives.

Materials Category/ Type
Sensors/Metals, Ceramics
High-chromia smart refractory materials, chromium (III) oxide brick

Manufacturing/Fabrication Process/Method
Printed/Laminated Tape Embedding, thermal processing, sintering

End Use: Sensors, gasification

Solid State Joining of Creep Enhanced Ferritic Steels

Performer: Pacific Northwest National Laboratory (PNNL)
Award Number: FWP-66059
Project Duration: 10/01/2014 – 09/30/2016
Total Project Value: $675,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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

Flat plate FS welds in HSLA65 plate, stay flat.

Materials Category/ Type
Materials/Alloys, Steels
Creep Strength Enhanced Ferritic steels, Gr91, Gr92, Gr122, P91, P92, P122, Boron/cobalt enriched 9Cr ferritic steel.

Manufacturing/Fabrication Process/Method
Solid state joining, friction stir welding

End Use: Boilers and tubing, Turbines

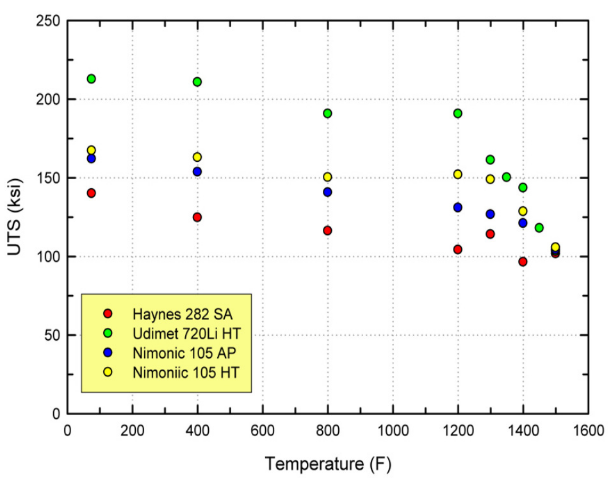
Plant Optimization Technologies

Steam Turbine Materials for Advanced Ultra Supercritical (AUSC) Coal Power Plants

Performer: Energy Industries of Ohio Inc.
Collaborator(s): ALSTOM Power Inc., Electric Power Research Institute, GE Energy Inc.
Award Number: FE0000234
Project Duration: 10/01/2009 – 09/30/2015
Total Project Value: $11,041,018
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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 AUSC conditions.

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



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

Materials Category/ Type:
Materials/Alloys
Nickel-base Blade/Bolting Candidate Alloys (617, 625, 263, 282, Nimonic 105, Haynes 282, Inconel 740, Udimet 720Li), Stellite6B, Tribaloy T-400C, Metco 45, CrC-NiCr, SHS 7170, SHS 9172, MoB-CoCr

Manufacturing/Fabrication Process/Method:
Pressure and vacuum casting, Argon oxygen decarburization, electric arc welding

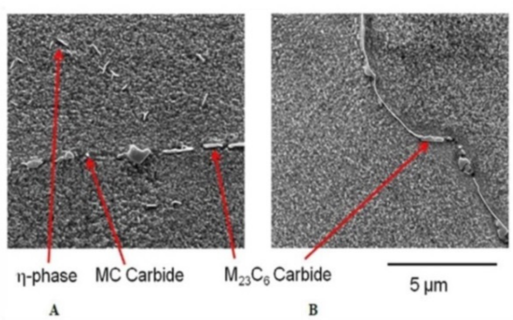
End Use: Turbines

Ultra-Supercritical Steam Cycle Turbine Materials

Performer: Oak Ridge National Laboratory - ORNL
Award Number: FWP-FEAA069
Project Duration: 10/01/2009 – 09/30/2016
Total Project Value: $2,250,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

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

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



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

Materials Category/ Type
Materials/Alloys
Nickel-based alloys, HR 282, HR 263, IN 740, Nimonic 105, Alloy 263

Manufacturing/Fabrication Process/Method
Casting, welding, joining

End Use: Turbines

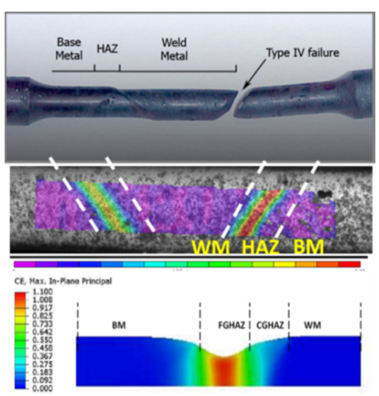
Weldability of Creep Resistant Alloys for Advanced Power Plants

Performer: Oak Ridge National Laboratory - ORNL
Award Number: FWP-FEAA118
Project Duration: 10/01/2013 – 09/30/2016
Total Project Value: $800,000
Technology Area: Plant Optimization Technologies
Key Technology: High Performance Materials

NETL is partnering with Oak Ridge National Laboratory on this project. This project aims to develop practical engineering solutions on two key issues on the weldability of high-temperature creep-resistant alloys used in advanced fossil energy power plants – (1) the reduced creep strength of the weld region vs. the base metal, and (2) welding of dissimilar metals.

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

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



(a) A crept sample showing Type IV failure in the HAZ of a cross-weld sample after 2500 hours of testing
(b) Full field creep strain measurement of Grade 91 steel cross-weld sample after 90 hours creep testing showing significant creep deformation localization in the HAZ that lead the HAZ failure. The measurement was by a specifically developed digital image correlation technique at ORNL.
(c) Feasibility demonstration of ICWE modeling of creep strain localization in cross-weld specimen after 13000 hours creep in this project

Materials Category/ Type
Materials/Alloys, Steels
Creep Strength Enhanced Ferritics, Austenite Stainless steels, Ni-Based Superalloys, Oxide Dispersion Strengthened Alloys

Manufacturing/Fabrication Process/Method
Computational welding modeling, rapid cooling, in-situ neutron and synchrotron experimental techniques, pre-weld heat treatments

End Use: Boilers and tubing, Turbines

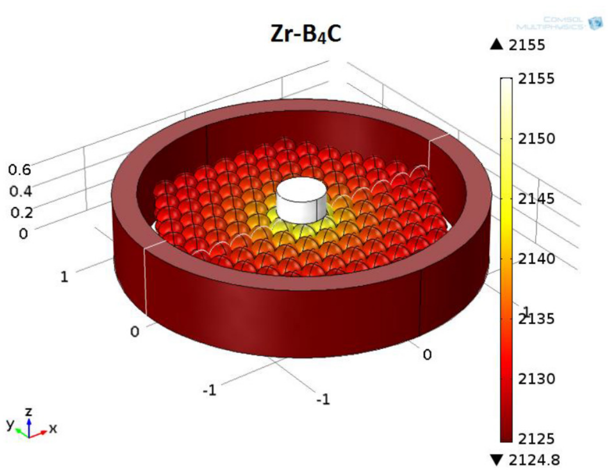
University Training and Research

Southern University and A&M College System	Novel Nano-Size Oxide Dispersion Strengthened Steels Development through Computational and Experimental Study	70
West Virginia University	Passive Wireless Sensors Fabricated by Direct-Writing for Temperature and Health Monitoring of Energy Systems in Harsh-Environments	71
Purdue University	Predicting Microstructure-Creep Resistance Correlation in High Temperature Alloys over Multiple Time Scales	72
Prairie View A&M University	Post Combustion Carbon Capture Using Polyethylenimine (PEI) Functionalized Titanate Nanotubes	73
University of Toledo	Processing and Evaluation of Next Generation Oxygen Carrier Materials for Chemical Looping Combustion	74
North Carolina State University	Rational Design of Mixed-Metal Oxides for Chemical Looping Combustion of Coal via Coupled Computational-Experimental Studies	75
University of Illinois	Serration Behavior of High-Entropy Alloys	76
Texas Engineering Experiment Station	Synergistic Computational & Microstructural Design of Next-Generation High-Temperature Austenitic Stainless Steels	77
University of Nebraska	Vertically-Aligned Carbon-Nanotubes Embedded in Ceramic Matrices for Hot Electrode Applications	78
University of Connecticut	Wireless 3D Nanorod Composite Arrays-Based High-Temperature Surface Acoustic Wave Sensors for Selective Gas Detection Through Machine Learning Algorithms	79

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: 07/01/2012 – 06/30/2015
Total Project Value: $200,000
Technology Area: University Training and Research
Key Technology: High Performance Materials

NETL is partnering with the University of Texas at El Paso to investigate computationally the plasma processing with strategic experimentation of SiC, ZrC-TiC-Y2O_3 and Ti_2AlC-TiC-Y_2O_3 packed beds, which ultimately will form SiO_2, ZrO_2-TiO_2- Y_2O_3, and Al_2O_3-Al_2TiO_5-Y_2O_3 scales for high temperature materials. The focus of the study is in understanding sufficiently plasma processing of nonmetallic packed beds for developing materials for extreme temperatures, such as materials with protective oxidizing scales operational at temperatures greater than 1773 kelvin (K). The plasma processing operating at 1973 to 2500 K for the carbides and their oxidation at 1973 K will involve the following research objectives: (1) investigate the effects of the plasma flow dynamics within the pores to form oxycarbide and amorphous phases, which ultimately would impede oxygen ingress through a packed bed or a protective scale; (2) determine the effect of the potential gradient established by the electromagnetic field on sealing pores as a result of the temperature spikes on pore surfaces; and (3) investigate the surface kinetics within the pore wall of the packed bed as a result of the plasma coupling mass and heat transport.



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

Materials Category/ Type:
Materials/Ceramics, Metals
SiO_2, ZrO_2-TiO_2-Y_2O_3, Al_2O_3-Al_2TiO_5-Y_2O_3

Manufacturing/Fabrication Process/Method:
Computational thermodynamics modelings, COMSOL multiphysics Simulation software, plasma processing

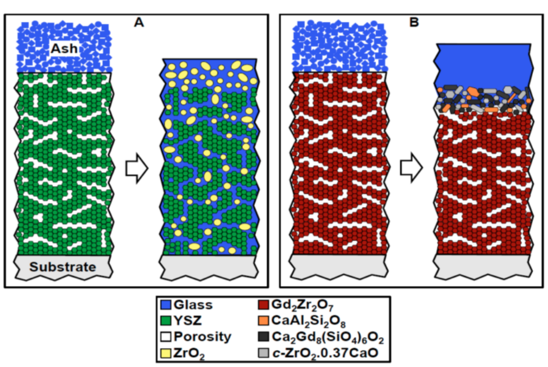
End Use: Boilers and tubing

Advanced Thermal Barrier Coatings for Next Generation Gas Turbine Engines Fueled by Coal-Derived Syngas High-Temperature Austenitic Stainless Steels

Performer: Brown University
Award Number: FE0008933
Project Duration: 09/01/2012 – 08/31/2015
Total Project Value: $324,400
Technology Area: University Training and Research
Key Technology: High Performance Materials

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.

Materials Category/ Type:
Coatings/Alloys, Substrates
Yttria stabilized zirconia (YSZ)

Manufacturing/Fabrication Process/Method:
Thermo-chemo-mechanical modeling, Ball milling, Air plasma spraying

End Use: Turbines

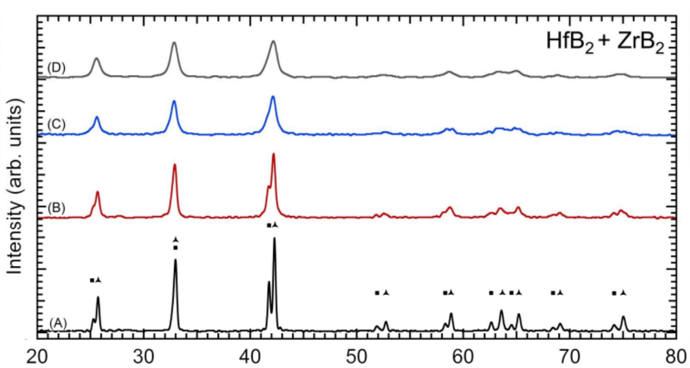
Boride Based Electrode Materials with Enhanced Stability under Extreme Conditions for MHD Direct Power Extraction

Performer: University of Idaho
Award Number: FE0022988
Project Duration: 07/01/2014 – 12/31/2017
Total Project Value: $ 399,938
Technology Area: University Training and Research
Key Technology: Innovative Energy Concepts

NETL is partnering with the University of Idaho to develop a boride-based ultrahigh temperature ceramic material that possesses all the required properties to function as sustainable electrodes in direct power extraction applications based on magneto-hydrodynamics (MHD). Transition metal borides display several unique properties including high melting point, high electrical and thermal conductivities, high strength and hardness even at elevated temperatures, and chemical stability.

In MHD direct power extraction, a hot conducting combustion flame flows through a transverse magnetic field and current is directly extracted. The conductivity of the flame is increased by addition of potassium salts as seed. The operating conditions of the MHD ducts are very aggressive due to high flame temperatures (~3000 K), high mass flow rate, and corrosive attack of the potassium salts. Oxide-based materials such as strontium doped $LaCrO_3$ have been considered candidate materials for the current-extracting electrodes. These conventional oxide materials show high electrical resistivity, low thermal conductivity, and high volatility at MHD operating temperatures, all of which limit their functionality.

The outcome of this project may lead to a better understanding of charge and mass transport behavior of transition metal borides and their oxidation kinetics in the presence of silicon and rare earth compounds. The results obtained from the project may help develop ultrahigh temperature electrode materials for MHD direct power extraction applications with improved lifetime and eventually the performance efficiency of coal-fired power plants.



X-ray powder diffraction patterns of the products after milling a (1:1) mixture of HfB_2 +ZrB_2 powder to ball ratio (1:20): (A) 5 minutes mill time, (B) 60 minutes mill time, (C) 180 minutes mill time, (D) 270 minutes mill time ■ ZrB_2 ▲HfB_2

Materials Category/ Type:
Coatings/Electrode
Metal Borides, ZrB_2, HfB_2, Salts

Manufacturing/Fabrication Process/Method:
Spark Plasma Sintering, Mechanochemical Synthesis, Electrochemical Anodization
Mechanical Milling

End Use: Boilers and tubing, turbines

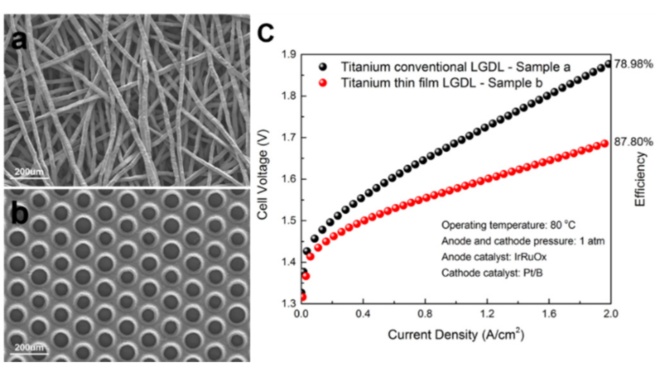
Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage

Performer: University of Tennessee
Collaborator(s): University of Tennessee Space Institute
Award Number: FE0011585
Project Duration: 09/01/2013 – 08/31/2016
Total Project Value: $470,084
Technology Area: University Training and Research
Key Technology: Innovative Energy Concepts

NETL is partnering with University of Tennessee to develop a thin and well-tunable multifunctional component 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.

The novel titanium liquid/gas diffusion layers (LGDLs) with well-tunable pore morphologies was developed by employing micro/nano-manufacturing and showed significant performance improvements in proton exchange membrane electrolyzer cells (PEMECs). As shown in Figure 1, the operating voltages required at a current density of 2.0 A/cm2 were as low as 1.69 V, and its efficiency reached a report high of up to 88%. In addition, the LGDL thickness reduction from 350 µm of conventional LGDLs to 25 µm will greatly decrease the weight and volume of PEMEC stacks, which can lead to new directions for future developments of low-cost PEMECs with higher performance. Its well-tunable features, including pore size, pore shape, pore distribution, and thus porosity and permeability, will be very valuable for developing PEMEC models and to validating simulations of PEMECs with optimal and repeatable performance.

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



(a) Conventional felt LGDL; (b) Novel thin LGDL; (c) Performance comparisons in the PEME

Materials Category/ Type
Materials/Metals
Titanium (Ti) Foils,

Manufacturing/Fabrication Process/Method
Computational modeling of Two-phase transport model in electrolyzers; physical and chemical vapor deposition, etching, Microfabrication and nanofabrication

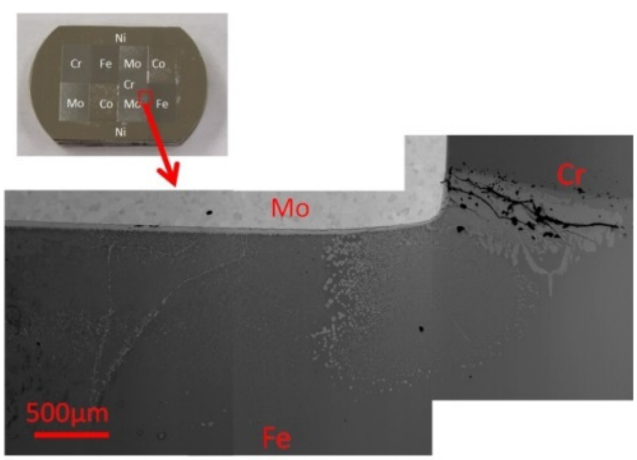
End Use: Energy storage

Effective Exploration of New 760 Degree Celsius Capability Steels for Coal Energy

Performer: Ohio State University Research Foundation
Award Number: FE0008960
Project Duration: 09/01/2012 – 08/31/2015
Total Project Value: $ 299,934
Technology Area: University Training and Research
Key Technology: High Performance Materials

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.

Materials Category/ Type:
Materials/Steels
Steel concentrations with high iron and chromium,

Manufacturing/Fabrication Process/Method:
Hot-Isostatic Pressing, Electron-Beam Welding, Grinding, Polishing

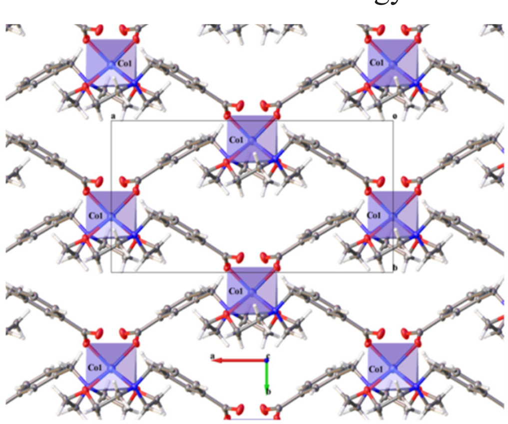
End Use: Boilers and tubing, turbines

Engineering Accessible Adsorption Sites in Metal Organic Frameworks for CO_2 Capture

Performer: Clark Atlanta University
Award Number: FE0022952
Project Duration: 10/01/2014 – 09/30/2017
Total Project Value: $ 249,998
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



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

Materials Category/ Type:
Materials/Metal powders

Manufacturing/Fabrication Process/Method:
X-ray crystallography, powder X-ray diffraction, thermogravimetric analysis, infrared spectroscopy

End Use

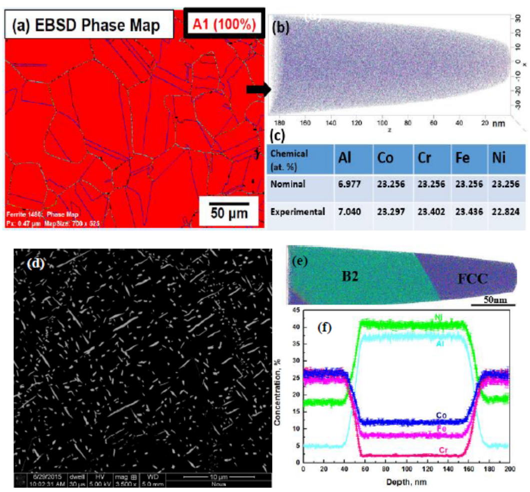
Capture from industrial processes; post-combustion capture

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

Performer: University of Tennessee
Collaborator(s): Computherm, LLC
Award Number: FE0008855
Project Duration: 08/01/2012 – 07/31/2015
Total Project Value: $300,000
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



(a) Electron BackScatter Diffraction (EBSD) phase map, (b) APT, and (c) Related chemical compositions of the $Al_{0.3}CoCrFeNi$ (as-HIPed); (d) SEM image, (e) APT, and (f) Related concentration profile of the $Al_{0.3}CoCrFeNi$ (annealed at 700°C for 500 h).

Materials Category/ Type:
Materials/Alloys
High-entropy alloys ($Al_xCrCuFeMnNi$)

Manufacturing/Fabrication Process/Method:
Vacuum arc casting, Neutron and synchrotron diffraction, Calculation of phase diagrams, differential thermal analysis, in-situ neutron diffraction

End Use: Boilers and tubing

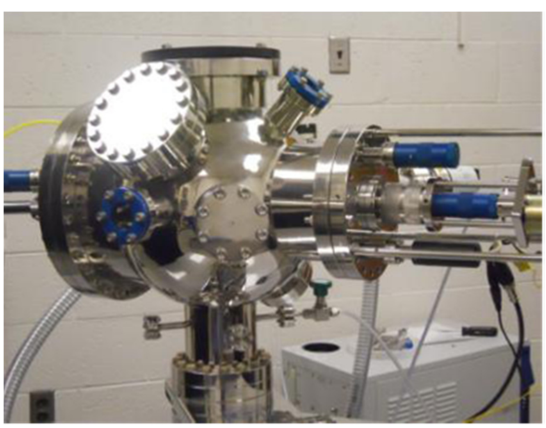
Gallium Oxide Nanostructures for High-Temperature Sensors

Performer: University of Texas at El Paso
Award Number: FE0007225
Project Duration: 10/01/2011 – 01/31/2015
Total Project Value: $200,000
Technology Area: University Training and Research
Key Technology: Sensors and Controls

This project was focused on the design of gallium oxide (Ga_2O_3)-based nanostructured materials capable of operating with demonstrated reliability and stability, and without significant interference from other pollutants or emissions, under the extreme conditions within fossil fuel energy systems. The experimental approaches and methods will address issues and technical barriers related to the growth, microstructure-property relationship, and ability to evaluate the performance of Ga_2O_3-based oxygen sensors.

The goal of this project was to develop high-temperature O_2 sensors, based on pure and doped Ga_2O_3 nanostructures, capable of operating at 800 °C and above in corrosive atmospheres. The specific objectives are (1) to fabricate high-quality pure and doped Ga_2O_3-based materials and optimizing conditions to produce unique architectures and morphology at the nanoscale; (2) to derive the structure-property relationships at nanoscale dimensions and demonstrate enhanced high-temperature oxygen sensing and stability; and (3) to promote research and education in the area of sensors and controls.

This project fostered the development of high-temperature O_2 sensors with enhanced selectivity, sensitivity, and long-term stability when compared to their conventional counterparts. Improved O_2 sensors will contribute to cleaner and more efficient coal-fired power generating plants.



Sputter Deposition System Developed by the Researchers

Materials Category/ Type:
Sensors/Oxides, Powders
Ga_2O_3 nanostructures, W-doped Ga_2O_3 nanostructures, GaN powders

Manufacturing/Fabrication Process/Method:
Conformal sputtering deposition, Physical vapor radio-frequency magnetron, Planetary ball and high-energy mechanical milling

End Use: Sensors

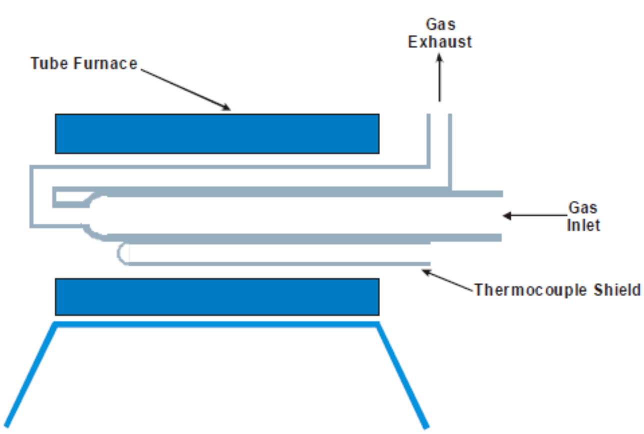
Graphene-based Composite Sensors for Energy Applications

Performer: West Virginia University Research Corporation
Award Number: FE0011300
Project Duration: 07/17/2013 – 07/16/2016
Total Project Value: $300,000
Technology Area: University Training and Research
Key Technology: Sensors and Controls

The objectives of this research are to develop and demonstrate the use of graphene-based composites as a high sensitivity, rapid response electronic nose for sensing gas species in energy applications. Graphene-based materials that support sensing structures in the temperature range of 600 °C - 1000 °C will be targeted. The scope of work includes (a) establishing procedures for controllable nucleation and growth of nanoparticles on graphene surface defects as a basis for selective gas sensing, (b) fabrication of graphene-based composite sensors, (c) fabrication of ruggedized deployable graphene-based composite sensors, (d) establishment of the electrical properties of graphene-based composites, (e) establishment of the characteristics of graphene-based composite sensors in simple mixtures, (f) establishment of the characteristics of graphene-based composite sensors in simulated environments, and (g) testing of the graphene-based sensors in representative environments and applications.

This work will focus on deriving, implementing, and testing agent-objective functions that promote coordinated behavior in large heterogeneous sensor networks. The long-term objective of the proposed work is to provide a comprehensive solution to the scalable and reliable sensor coordination problem to lead to safe and robust operation of advanced energy systems.

The objectives support this goal by first ensuring that the information collected by the heterogeneous sensors provides the greatest added value to the full network, and then by ensuring that that information can be effectively used to improve advanced power system performance. The method will be tested to ensure robust network operation and good response to system change.



Experimental setup for rapid thermal annealing.

Materials Category/ Type
Sensors/Metals, Substrates
Graphene-based Nanoparticle Composites, G/SiC, 4H-SiC Substrates, 6h-SiC Substrates, Ag, Au

Manufacturing/Fabrication Process/Method
Rapid Thermal Annealing and Ultrahigh Vacuum Annealing, Etching

End Use: Sensors, gasification, boilers and tubing

University Training and Research

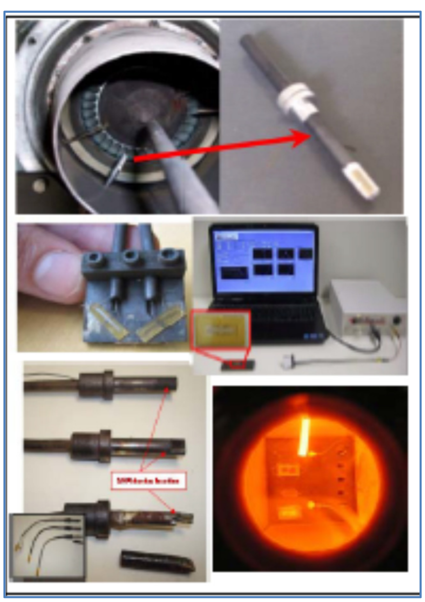
High Temperature Integrated Gas and Temperature Wireless Microwave Acoustic Sensor System for Fossil Energy Applications

Performer: University of Maine System
Award Number: FE0026217
Project Duration: 09/01/2015 – 08/31/2018
Total Project Value: $399,999
Technology Area: University Training and Research
Key Technology: Sensors and Controls

This project aims to develop a wireless integrated gas/temperature microwave acoustic sensor capable of passive operation (no batteries) over the range 350 - 1000 °C in harsh environments relevant to fossil energy technology, with specific applications to coal gasifiers, combustion turbines, solid oxide fuel cells, and advanced boiler systems.

The proposed wireless sensor system is based on a surface acoustic wave (SAW) sensor platform that could be used to detect H_2, O_2, and NOX gases and monitor the gas temperature in the harsh environment. Fully packaged prototype sensors will be designed, fabricated, and tested under gas flows of H_2 (< 5%), O_2, and NOX in laboratory furnaces, and the sensor response characterized for sensitivity, reproducibility, response time, and reversibility over a range of gas temperatures.

The SAW sensors have the advantage of being potentially readily scalable for rapid manufacturing using photolithography/metallization fabrication steps, followed by integration of each sensor into a stand-alone wireless harsh environment sensor package. The SAW gas sensor technology will be targeted for demonstration and implementation in a power plant environment. Acquiring temperature and gas composition data from wireless sensors at diverse harsh environment locations in power plants will aid in increasing fuel burning efficiency, reduce gaseous emissions, and reduce maintenance costs through condition-based monitoring.



Example of UMaine harsh environment wireless LGS SAW sensors

Materials Category/ Type:
Materials/Ceramics, Metals/Alloys

Manufacturing/Fabrication Process/Method:
Photolithography; thin film deposition

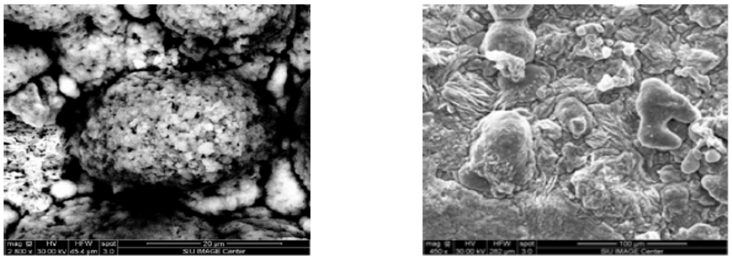
End Use: Pulverized Coal Combustion, IGCC, SOFC

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: 09/01/2012 – 08/31/2015
Total Project Value: $442,212
Technology Area: University Training and Research
Key Technology: High Performance Materials

NETL is partnering with Southern Illinois University to develop TiC- and TiB_2-based coatings applied via high velocity oxygen fuel (HVOF) thermal spray method onto various substrates used in boilers and turbines operating under ultrasupercritical steam conditions. The specific objectives of the project are (1) synthesis of nanoparticles of TiC by a patented process, (2) extension of the process to synthesize nanosized 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 waterwall 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)

Materials Category/ Type:
Coatings/Alloys
Titanium Carbide, Titanium Boride, Nickel Alloy

Manufacturing/Fabrication Process/Method:
High velocity oxygen fuel thermal spray

End Use: Boilers and tubing, Turbines

University Training and Research

Investigation on Pyroelectric Ceramic Temperature Sensors for Energy System Applications

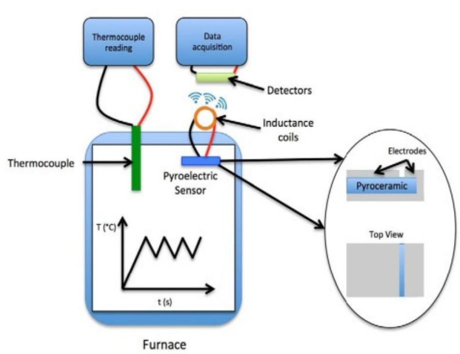
Performer: University of Texas at El Paso
Award Number: FE0011235
Project Duration: 07/01/2013 – 06/30/2016
Total Project Value: $200,000
Technology Area: University Training and Research
Key Technology: Sensors and Controls

The research team will fabricate pyroelectric ceramic films using an electrophoretic deposition process and characterize their material properties such as microstructure, morphology, and crystal structure. Pyroelectric materials generate an electric charge upon a change in temperature, and it is this effect upon which the sensor is based. Deposition by electrophoresis—the motion of dispersed particles in a fluid under uniform electric charge—has many advantages and may be achieved by a number of methods.

The wireless sensor system will be constructed using a pyroceramic and inductive coupling technique, where the current generated by the pyroceramic will, upon a change in temperature, be converted to magnetic flux that is wirelessly detected by an inductance coil. Before applying this wireless sensor system to energy systems, it will be calibrated using a commercial thermocouple as a reference. Finally, the research team will conduct torch and combustor rig testing to determine the sensor's ability to function in the energy system. A full report of the sensor's design, fabrication process, and characterization method will be delivered upon completion of the project.

The goal of the project is to develop a self-powered, low-cost wireless temperature sensor capable of withstanding harsh environments. The objectives are fabrication and characterization of pyroelectric ceramic temperature sensor materials, construction of a wireless sensing system and demonstration of its temperature sensing capability, and demonstration of wireless temperature sensing and other requisite capabilities, including data transmission and durability, at the high temperatures and harsh environmental conditions of coal-based power systems.

The proposed work may result in the development of a low-cost, reliable, extremely sensitive, high-temperature, harsh environment sensor that will help increase the affordability and efficiency and reduce emissions of advanced power plants. Additionally, participating students will receive training in the development of pyroelectric ceramic temperature sensor materials under this Historically Black Colleges and Universities research program.



Calibration and Demonstration of wireless temperature sensing.

Materials Category/ Type:
Sensors/Ceramics, Oxides
Pyroelectric ceramics, $LiNbO_3$

Manufacturing/Fabrication Process/Method:
Electrophoretic Deposition

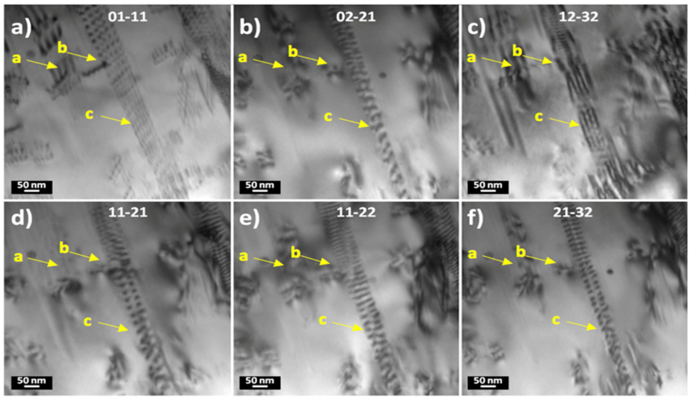
End Use: Sensors

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

Performer: Dartmouth College
Award Number: FE0008857
Project Duration: 09/01/2012 – 08/31/2015
Total Project Value: $402,467
Technology Area: University Training and Research
Key Technology: High Performance Materials

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



TEM image of dislocations and stacking faults in a Laves phase precipitate after high temperature deformation.

Materials Category/ Type
Materials/Alloys, Steels
Aluminum-alloyed Laves phase-strengthened austenitic steel (Fe-32Ni-14Cr-3Nb-3Al-3Ti-0.3Zr-0.15Si)

Manufacturing/Fabrication Process/Method
Thermo-mechanical processing, Cold rolling

End Use: Boilers and tubing

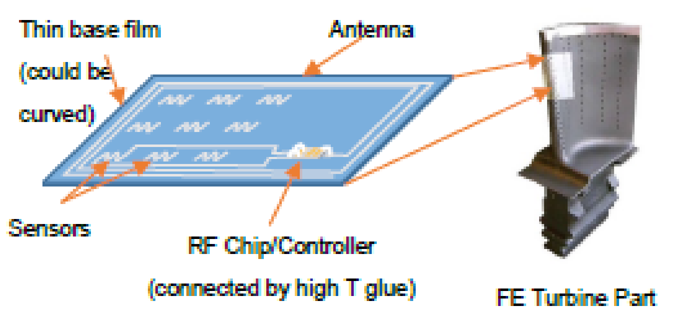
Low-Cost Efficient and Durable High Temperature Wireless Sensors by Direct Write Additive Manufacturing for Application in Fossil Energy Systems

Performer: Washington State University
Collaborator(s):
Award Number: FE0026170
Project Duration: 10/01/2015 - 09/30/2018
Total Project Value: $488,738
Technology Area: University Training and Research
Key Technology: Sensors and Controls

This project will design, characterize, and demonstrate wireless, conformal strain and pressure sensors manufactured using low-cost, direct write additive methods for application in fossil energy (FE) systems. The goal is to demonstrate the feasibility of 'low-cost aerosol jet manufacturing' for FE systems and to develop next-generation sensors and controls, which can sustain high temperatures up to 500 °C.

Specifically, this project will advance the current state of the art by developing novel materials and devices for wireless circuits that surpass 350 °C, the operating temperature limits of traditional silicon-based electronics; integrating electronic circuitry on curved 3-D surfaces such as those observed in gas turbine engines, demonstrating capabilities that surpass that of traditional (2-D) lithographic techniques; and improving reliability issues for wireless sensors that arise from the demanding FE environments.

It is anticipated that this reseach could improve the in-situ monitoring and thus the performance of the FE devices and systems.



Schematic of a fully integrated high temperature wireless sensor system

Materials Category/ Type Sensors **Manufacturing/Fabrication Process/Method** Aerosol Jet Micro-Additive Manufacturing (AJ-MAM)
End Use
Oxy-fuel Combustion; Chemical Looping Combustion

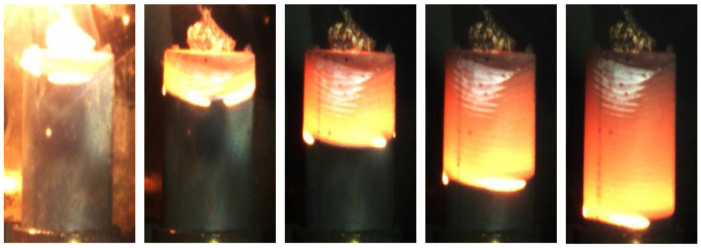
University Training and Research

Mechanically Activated Combustion Synthesis of $MoSi_2$-Based Composites

Performer: University of Texas at El Paso
Award Number: FE0008470
Project Duration: 07/01/2012 – 09/30/2015
Total Project Value: $236,000
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



Spin combustion of Mo-Si-B mixture.

Materials Category/ Type
Materials/Ceramics
Molybdenum Disilicide ($MoSi_2$) Based Composites

Manufacturing/Fabrication Process/Method
Compaction, High-energy ball milling, Mechanically activated self-propagating high-temperature synthesis

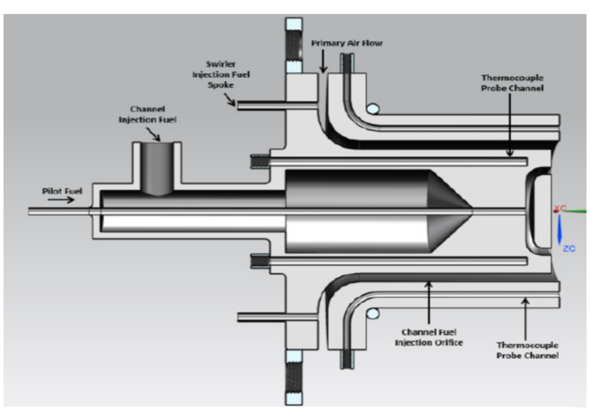
End Use: Boilers and tubing

Metal Three Dimensional (3D) Printing of Low-Nitrous Oxide (NO_X) Fuel Injectors with Integrated Temperature Sensors

Performer: University of Texas at El Paso
Collaborator(s):
Award Number: FE0026330
Project Duration: 10/01/2015 - 09/30/2018
Total Project Value: $ 250,000
Technology Area: University Training and Research
Key Technology: Sensors and Controls

This work necessitates the exploration of design and prototyping of a Dry Low-NOX (DLN) fuel injector with integrated temperature sensing capabilities using the electron beam melting (EBM) additive manufacturing (AM) process. Low-NOx natural gas fuel injectors, commonly used in Dry Low NOx (DLN) gas turbine combustors, have complex internal cavities and passages to ensure tailored mixing of air and fuel to achieve ultra-low levels of NOX emission. Since the current design methodology of these injectors is based on conventional fabrication techniques (e.g. multi-step machining and welding processes), a new paradigm of design methodology needs to be developed for their adaptation to the EBM fabrication process.

The proposed effort has three specific objectives: (1) development of design methodologies for Low-NOx fuel injectors with embedded temperature capabilities for EBM based 3D Manufacturing; (2) development of optimum EBM process parameters and powder removal techniques to remove sintered powder from internal cavities and channels of Low-NOx fuel injectors with embedded temperature sensors; and (3) Testing of the EBM fabricated Low-NOx fuel injector with integrated temperature measurement capabilities in a high-pressure laboratory turbine combustor. Metal AM processes allow embedding or integrating sensors in complex energy system components without post-production modification of the component. Conventional manufacturing processes generally require more than five steps of fabrication, assembly, and finishing to develop energy system components such as fuel injectors with complex internal geometries. In contrast, the same part can be fabricated in a single metal AM step with the option of sensor integration and more complex internal geometries.



Test Article to be Designed and Fabricated: Dry Low NOx Fuel Injector with integrated Ceramic Insulated High Temperature Thermocouples

Materials Category/ Type
Materials/alloys - Inconel 718, Inconel 625, and/or Titanium

Manufacturing/Fabrication Process/Method
Additive manufacturing (AM) fabrication process - electron beam melting (EBM))

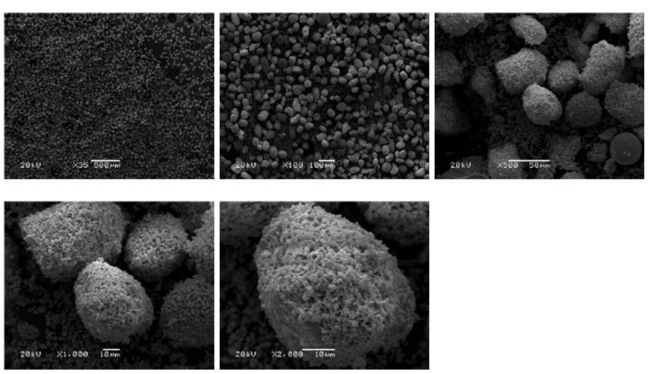
End Use
Gas turbines

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

Performer: Trustees of Indiana University
Award Number: FE0008868
Project Duration: 09/01/2012 – 08/31/2015
Total Project Value: $293,519
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



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

Materials Category/ Type:
Coatings/Alloys, Ceramics, Oxides
Ni-based superalloy , Pyrochlore Oxide, $La_2Zr_2O_7$, Zirconate Ceramics, NiCoCrAlY Bond Coat Alloy, $Nd_2Zr_2O_7$, $Sm_2Zr_2O_7$, $Gd_2Zr_2O_7$, CoNiCrAlY

Manufacturing/Fabrication Process/Method:
High Velocity Oxygen Fuel Thermal and Air Plasma Spraying

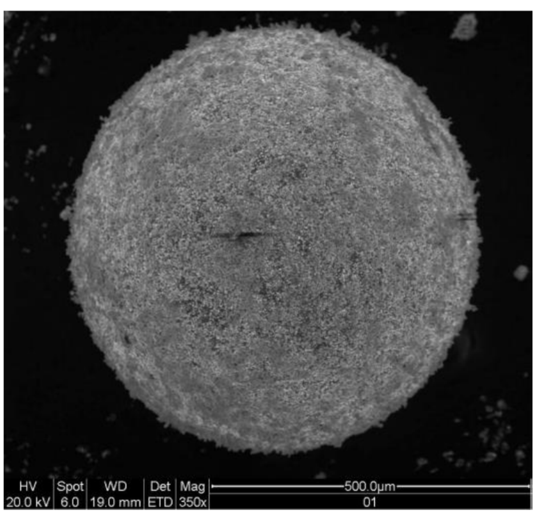
End Use: Turbines

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

Performer: Howard University
Collaborator(s): The Ohio State University
Award Number: FE0011515
Project Duration: 07/01/2013 – 06/30/2015
Total Project Value: $199,892
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



Materials Category/ Type
Materials/Sorbents, alloys, metals, oxides Fe2O3-shell micro-particles, Al2O3-core micro-particles, CaO-core/Fe2O3-shell particle

Manufacturing/Fabrication Process/Method
Vapor deposition, Mechanical granulation, Cyclic oxidation and Reduction

End Use:
Carbon capture, chemical

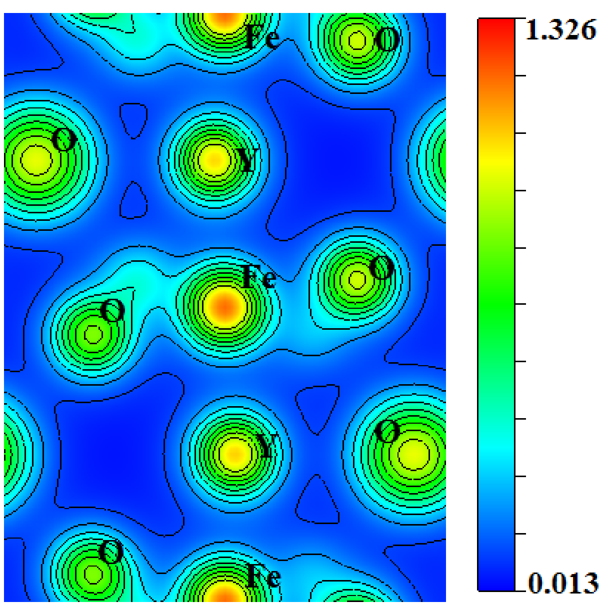
Novel Nano-Size Oxide Dispersion Strengthened Steels Development through Computational and Experimental Study

Performer: Southern University and A&M College
Award Number: FE0008382
Project Duration: 06/01/2012 – 02/28/2016
Total Project Value: $200,000
Technology Area: University Training and Research
Key Technology: High Performance Materials

NETL partnered with Southern University to identify—through ab initio molecular dynamics atomic level modeling and computer simulation—and experimentally validate new oxide dispersion strengthened (ODS) steel alloy compositions that have improved high temperature mechanical and corrosion resistance properties for advanced fossil energy applications. These tools simulate and determine key properties of new ODS alloy compositions.

The project team has studied iron/oxide interface through density functional theory and ab initio molecular dynamics simulation. Based on the simulation results, further studies of the elastic, phonon, and thermal stability of $YCrO_3$, $YCrO_4$, and $YFeO_3$ were conducted. In addition, both elastic, phonon, and thermal stability simulation and high-temperature and high-pressure experimental validation were performed. Final experimental confirmation of oxidation and corrosion resistance will be performed. The metal/oxide interface properties from both simulation and experimental characterization will be summarized and reported.

Two students from this Historically Black Colleges and Universities (HBCU) designated institution have been trained in materials modeling and high performance computing (HPC) simulation. They were also trained in the use of efficient analysis tools to process data. The unique integrated simulation and experimental methods used have assisted in optimizing high quality ODS compositions for high-temperature applications such as oxidation and corrosive resistance.



2D charge density contour in plane (001) of $FeYO_3$.

Materials Category/ Type
Materials/Alloys, Powders, Steels

Ferritic Oxide Dispersion Strengthened (ODS) Steel Alloys, Nano-scale Powders, Yttrium, Chromium, FeCrAl alloys, ODM751, MA956

Manufacturing/Fabrication Process/Method
Computational modeling of Interface energy, Ab Initio Molecular Dynamics, and Monte Carlo HPC Simulations

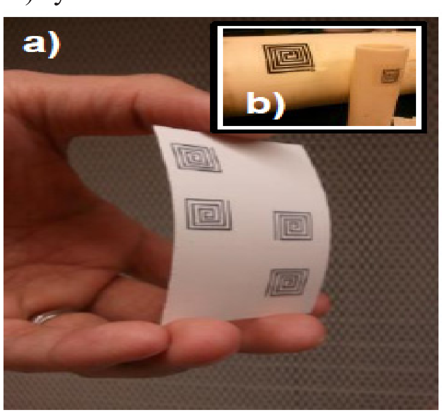
End Use: Boilers and tubing, turbines

Passive Wireless Sensors Fabricated by Direct-Writing for Temperature and Health Monitoring of Energy Systems in Harsh-Environments

Performer: West Virginia University
Collaborator(s): NexTech Materials, Ltd., General Electric Global Research
Award Number: FE0026171
Project Duration: 10/01/2015 - 09/30/2018
Total Project Value: $399,965
Technology Area: University Training and Research
Key Technology: Sensors and Controls

This project will demonstrate a wireless, high-temperature sensor system for monitoring the temperature and health of energy-system components. The active sensor and electronics for passive wireless communication will be composed entirely of electroceramic materials (conductive ceramics), which can withstand the harsh environments of advanced fossil-energy-based technologies. The project will focus primarily on the fabrication and testing of temperature (thermocouples and thermistors) and health (strain/stress and crack propagation sensors) that function at extreme temperatures (up to 500-1700 °C). A passive wireless communications circuit to accompany the high-temperature sensor that will allow the transmission of the data based on electromagnetic coupling to a near-by reader antenna will be developed along with a peel-and-stick-like transfer process to deposit the entire sensor circuit to various energy-system components.

The results of this research could reduce the need for interconnect wires near the active—and possibly rotating—energy-system component. It may also permit the economical and precise placement of the sensor circuit onto components of various shapes and locations, without altering the geometry and active features of the manufactured component, or necessitating the removal (or decommissioning) of the component for installation. The sensor system developed may find application in solid oxide fuel cells, chemical reactors, furnaces, engines, boilers, and gas turbines (for both energy and aerospace applications) systems.



a) Picture of spiral inductor pattern ink-jet printed of ceramic ink onto fugitive carrier film, and **b)** picture of two patterns transferred to alumina tubes by WVU's peel-and-stick process.

Materials Category/ Type
Sensors

Manufacturing/Fabrication Process/Method
2D/3D Direct-writing

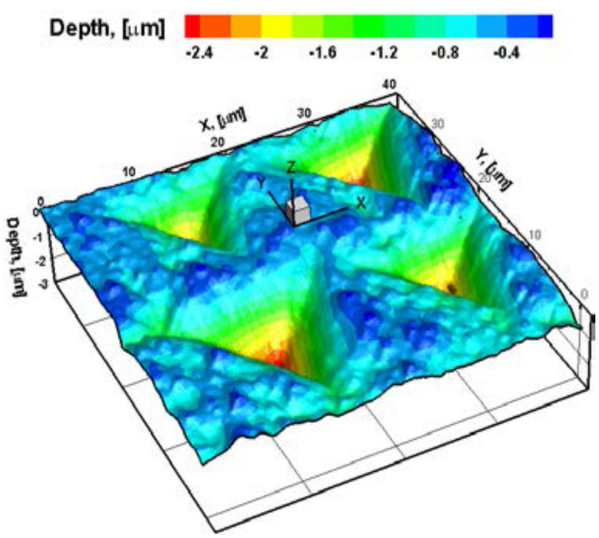
End Use
Solid oxide fuel cells, chemical reactors, furnaces, engines, boilers, and gas turbines

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

Performer: Purdue University
Collaborator(s): University of California - San Diego
Award Number: FE0011291
Project Duration: 07/22/2013 – 07/21/2016
Total Project Value: $300,000
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



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

Materials Category/ Type
Materials/Alloys
Refractory alloys, W-based Binary alloy, W-based Ternary Alloy, W-based body-centered-cubic (BCC) alloys, Ni, Pd, Co, Fe, Cu, binary Ni-W alloys (W-Ni, nanocrystalline pure Ni and Ni-W)

Manufacturing/Fabrication Process/Method
Cold Compaction, Ball Milling, Calculation of Phase Diagrams, Activated Sintering

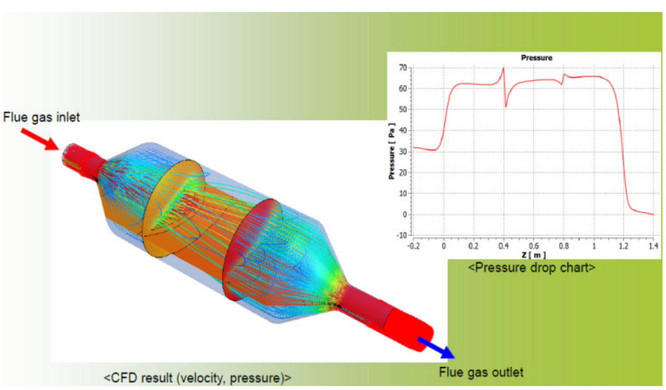
End Use: Boilers and tubing, gasification

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

Performer: Prairie View A&M University
Award Number: FE0023040
Project Duration: 10/01/2014 – 09/30/2017
Total Project Value: $ 249,996
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



CFD Modeling: Porous Media
Courtesy of Prairie View A&M University

Materials Category/ Type
Materials/Sorbents
Titanate (TiO2), Polyethylenimine (PEI),

Manufacturing/Fabrication Process/Method
Computational Fluid Dynamics Simulation; Thermogravimetric Analysis,

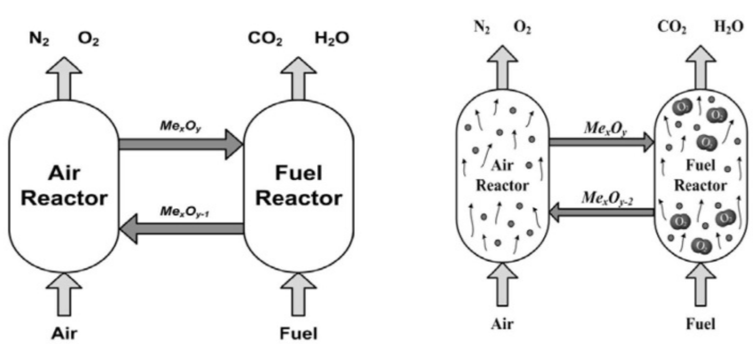
End Use: Boilers and Tubing, carbon capture

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

Performer: University of Toledo
Award Number: FE0008774
Project Duration: 09/04/2012 – 09/03/2016
Total Project Value: $470,674
Technology Area: University Training and Research
Key Technology: High Performance Materials

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.

Materials Category/ Type:
Materials/Oxides
ABO_3 and $A_2B_2O_6$ Perovskite Crystal, $CaMnO_3$

Manufacturing/Fabrication Process/Method:
Crushing, Dyeing, Mechanized homogenization, Milling,

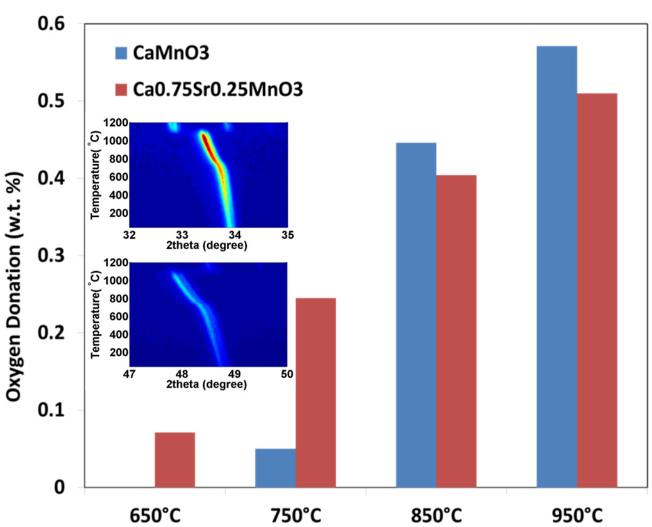
End Use: Chemical looping combustion

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

Performer: North Carolina State University
Award Number: FE0011247
Project Duration: 09/15/2013 – 09/14/2016
Total Project Value: $363,404
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



Sr-doped CaMnO3 perovskites showing superior oxygen uncoupling properties and redox stability

Materials Category/ Type
Materials/Oxides
Mixed Mn-Fe and Co-Fe oxides, perovskite, and perovskite composites

Manufacturing/Fabrication Process/Method
ab-initio/DFT and molecular dynamics (MD) simulations, genetic algorithm for material screening

End Use: Chemical looping combustion

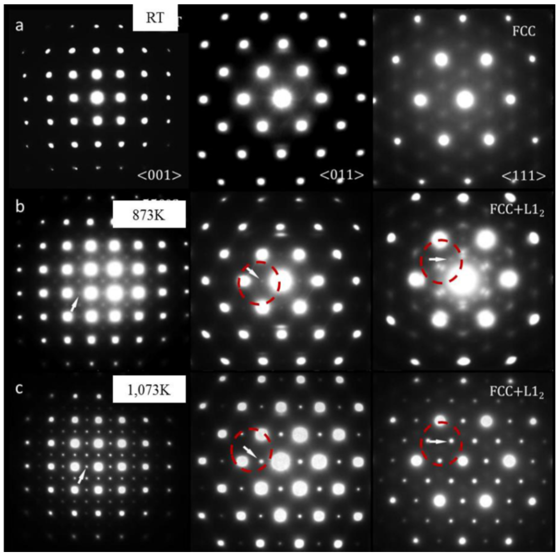
University Training and Research

Serration Behavior of High-Entropy Alloys

Performer: University of Illinois
Collaborator(s): The University of Tennessee
Award Number: FE0011194
Project Duration: 10/01/2013 – 09/30/2016
Total Project Value: $300,000
Technology Area: University Training and Research
Key Technology: High Performance Materials

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.



Selected-area-electron-diffraction patters of the deformed samples at a) TEM image at room temperature; b) 873 K; and c) 1,073 K

Materials Category/ Type;
Materials/Alloys
High-entropy alloys

Manufacturing/Fabrication Process/Method:
Statistical noise analysis, compression, Computational thermodynamics, Mean-field theory model

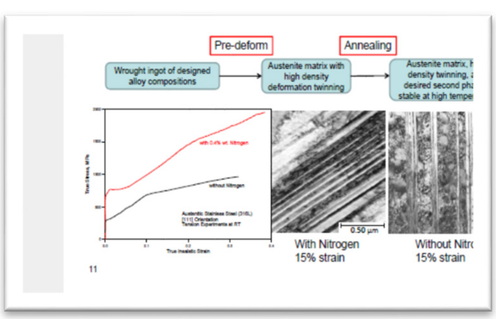
End Use: Boilers and tubing, Turbines

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

Performer: Texas Engineering Experiment Station
Award Number: FE0008719
Project Duration: 08/01/2012 – 07/31/2015
Total Project Value: $300,000
Technology Area: University Training and Research
Key Technology: High Performance Materials

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

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



Simple thermo-mechanical

Materials Category/ Type:
Materials/Alloys, Steels

Manufacturing/Fabrication Process/Method:
Micro-alloying, Equal channel angular pressing, Thermo-mechanical processing, Cold/hot rolling, Uniaxial tensioning, Twinning-induced grain boundary engineering

End Use: Boilers and tubing

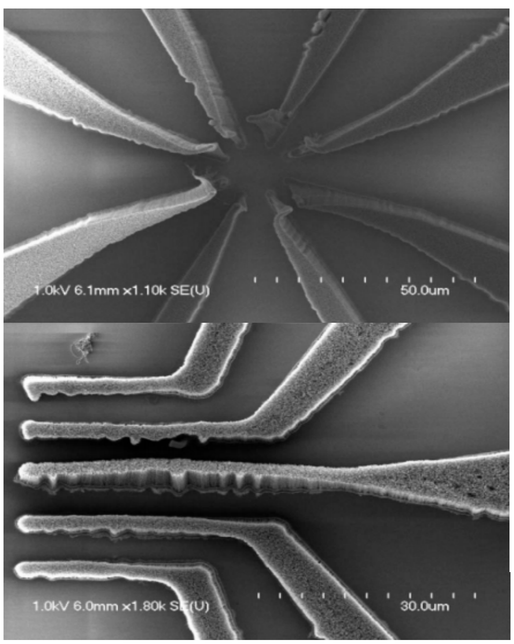
University Training and Research

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

Performer: University of Nebraska
Award Number: FE0023061
Project Duration: 10/01/2014 – 09/30/2017
Total Project Value: $ 400,000
Technology Area: University Training and Research
Key Technology: Innovative Energy Concepts

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

The successful development of the CNT-C composite structures will reduce the capital costs of the MHD power systems and establish a new family of VA-CNT-based anisotropic composite structures.



Vertically aligned CNT patterns

Materials Category/ Type
Materials/Ceramics, Metals
Cu substrate, CNT-Ceramic Composite Structures

Manufacturing/Fabrication Process/Method
Laser Direct Writing, Modulated photothermal radiometric method, Thermionic emission current method, Rapid thermal annealing, Sputtering, Deposition,

End Use:

Boilers and Tubing, turbines

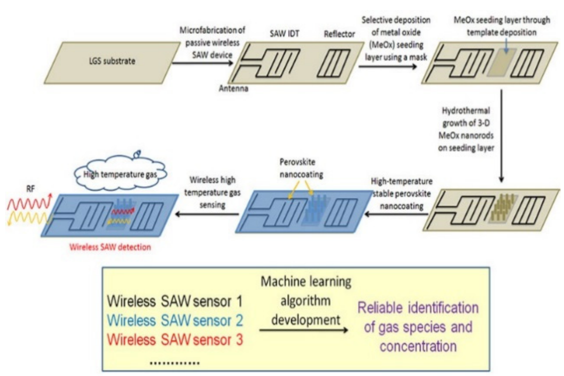
University Training and Research

Wireless 3D Nanorod Composite Arrays-Based High-Temperature Surface Acoustic Wave Sensors for Selective Gas Detection Through Machine Learning Algorithms

Performer: University of Connecticut
Collaborator(s):
Award Number: FE0026219
Project Duration: 09/01/2015 - 08/31/2018
Total Project Value: $400,000
Technology Area: University Training and Research
Key Technology: Sensors and Controls

This project aims at developing a wireless integrated gas/temperature microwave acoustic sensor capable of passive operation (no batteries) over the range of 350 °C to 1,000 °C in harsh environments relevant to fossil energy technology, with specific applications to coal gasifiers, combustion turbines, solid oxide fuel cells, and advanced boiler systems. The proposed wireless sensor system is based on a surface-acoustic-wave sensor platform that is configured using a langasite piezoelectric crystal with Pt/Pd interdigital electrodes and yttria-stabilized zirconia films doped with Pd, Pt, or Au nano-catalysts to detect H_2, O_2, and NO_X gases and to also monitor the gas temperature in the harsh environment. Fully packaged prototype sensors will be designed, fabricated, and tested under gas flows of H_2 (< 5 percent), O_2, and NO_X in laboratory furnaces, and the sensor response will be characterized for sensitivity, reproducibility, response time, and reversibility over a range of gas temperatures.

This project could advance development of high temperature stable sensing materials by developing a novel high-temperature sensing strategy to realize fast, sensitive, selective, rugged, and cost-effective high-temperature gas sensors for power and fuel systems. The sensing technique developed could be suitable for various fossil energy end-use applications ranging from ultra-supercritical boilers (up to 760 °C) to solid oxide fuel cells (650-1000 °C) and automotive engines (up to 1000 °C).



The wireless high-temperature surface-acoustic-wave gas sensor arrays with machine learning algorithm development

Materials Category/ Type:
Ceramic - oxides, Metals
Sensors

Manufacturing/Fabrication Process/ Method:
Pulsed laser deposition, magnetron sputtering, sol-gel wash coating

End Use:
Coal gasifiers, combustion turbines, solid oxide fuel cells, and advanced boiler systems cycles - AUSC.

University Training and Research

Abbreviations

3-D	three dimensional
AM	advanced manufacturing
AMNPO	Advanced Manufacturing National Program Office
AMP	Advanced Manufacturing Partnership
ASME	American Society of Mechanical Engineers
AUSC	advanced ultrasupercritical
C	Celsius
CCSI	Carbon Capture Simulation Initiative
CFD	computational fluid dynamic
CLC	chemical-looping combustion
CLOU	chemical-looping with oxygen uncoupling
CNT	carbon nanotubes
CSEF	creep strength enhanced ferritic steels
CVD	chemical vapor deposition
DOE	Department of Energy
DTA	differential thermal analysis
ECMD	electrically conductive membrane distillation process
EDF	erbium doped fiber
F	Fahrenheit
FBG	fiber bragg grating
FE	Fossil Energy
FGD	flue gas desulfurization
FO	fiber optic
FPI	Fabry-Perot interferometer
FSW	friction stir welding
GB	grain boundary
HBCU	Historical Black Colleges and Universities
HEAs	high-entropy alloys

HIP	hot isostatic pressure
HUMS	Health-Utilization Monitoring System
HVOF	high velocity oxygen fuel
ICWE	integrated computational weld engineering modeling tool
IGF	intergranular films
K	kelvin
kW_{th}	kilowatt thermal
L-BPF	laser powder bed fusion
LM	laser micromachining
LOM	laminated object manufacturing technique
MASHS	mechanically activated self-propagating high-temperature synthesis
MCCC	Metal-ceramic coaxial cable
MD	membrane distillation
MHD	magneto-hydrodynamic
MOCVD	metal organic chemical vapor deposition
MPa	megapascals
NDE	nondestructive evaluation
NETL	National Energy Technology Laboratory
NNMI	National Network for Manufacturing Innovation
NRAP	National Risk Assessment Partnership
NSTC	National Science and Technology Council
OC	oxygen carriers
OCMI	optical carrier-based microwave interferometry
ODS	oxide dispersion-strengthened
OMI	Other Minority Institutions
PM	powdered metal
psi	pounds per square inch
PWHT	post-weld heat treatment
R&D	Research and Development

RF	radio frequency
SBIR	Science Small Business Innovation Research Program
SOFC	solid oxide fuel cell
SPS	spark plasma sintering
TBC	thermal barrier coating
TDS	total dissolved solids
TE	thermoelectric
TEM	transmission electron microscopy
TG-DTA	thermogravimetric
TMC	transport membrane condenser
UCR	University Coal Research
USC	ultrasupercritical
UTR	University Training and Research
VA	vertically aligned

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