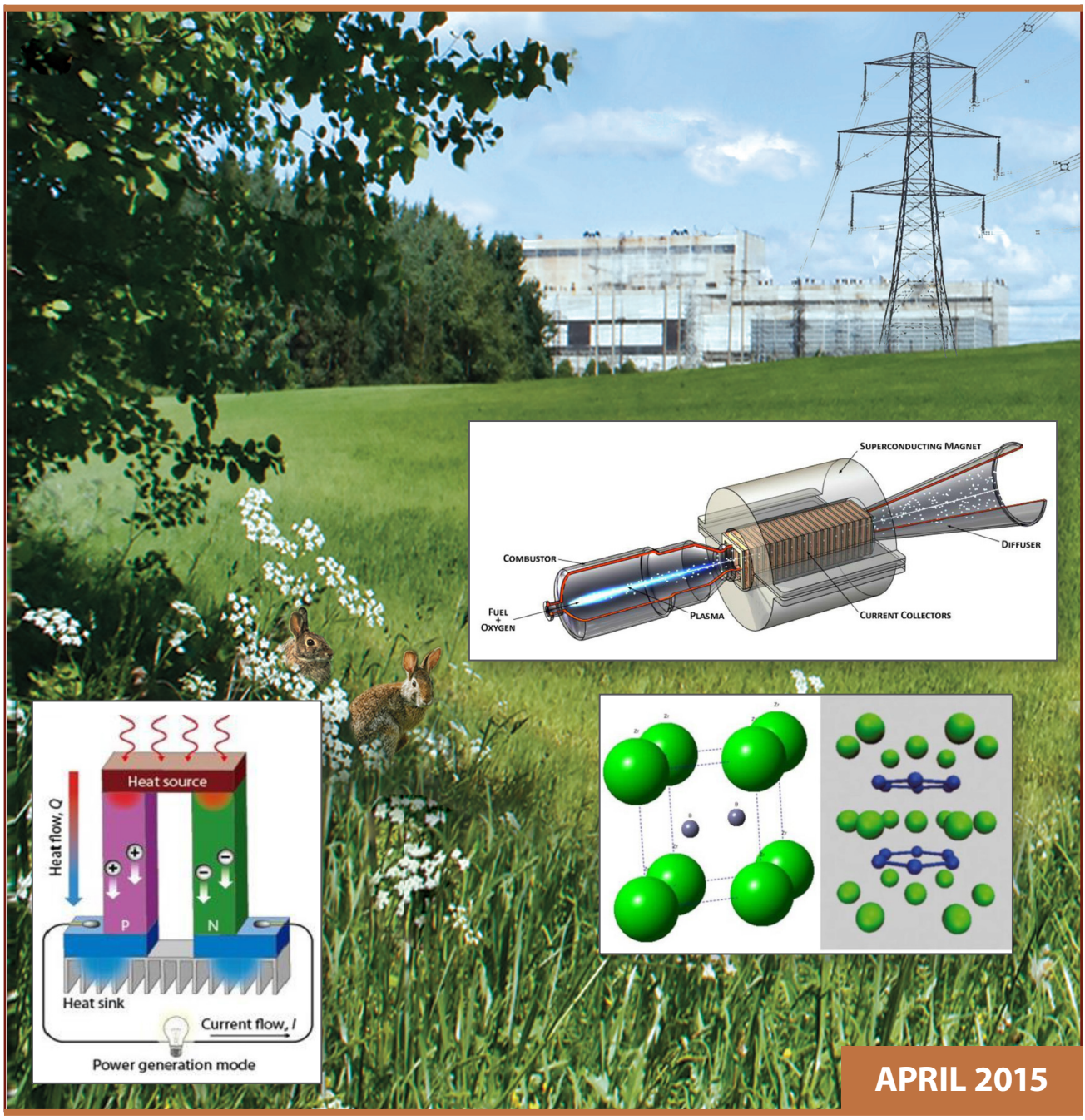
the ENERGY lab

Crosscutting Technology Research Innovative Energy Concepts Project Portfolio



APRIL 2015

U.S. DEPARTMENT OF ENERGY

the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

Disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Contents

Introduction 4

INNOVATIVE ENERGY CONCEPTS 6

University of Washington: High Temperature Thermoelectric Oxides Engineered at Multiple Length Scales for Energy Harvesting 7

University of Tennessee, Knoxville: Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage 8

University of Idaho: Boride Based Electrode Materials with Enhanced Stability under Extreme Conditions for MHD Direct Power Extraction 9

University of Nebraska: Vertically-Aligned Carbon-Nanotubes Embedded in Ceramic Matrices for Hot Electrode Applications. 10

University of Washington: Precursor-Derived Nanostructured Silicon Carbide Based Materials for Magnetohydrodynamic Electrode Applications 11

West Virginia University Research Corporation: Ceramic High Temperature Thermoelectric Heat Exchanger and Heat Recuperators in the Power Generation Systems 12

University of Texas at El Paso: High Temperature High Velocity Direct Power Extraction Using an Open Cycle Oxy Combustion System 13

National Energy Technology Laboratory - ORD: Innovative Process Technologies (Task4: Innovative Energy Concepts) 14

Abbreviations 15

Contacts 15

Acknowledgements 15

Introduction

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

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

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

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

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

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

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

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

The Crosscutting Technology Research program comprises these key technology areas:

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

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

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

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

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

Innovative Energy Concepts

Innovative Energy Concepts (IEC) is concerned with the development of innovative cost-effective technologies that promote efficiency, environmental performance, availability of advanced energy systems, and the development of computational tools that shorten development timelines of advanced energy systems. NETL is working with stakeholders to focus on two research areas:

- **Advanced Power Generation Concepts** such as direct power extraction, thermoelectric generation, and other innovative ideas have the potential to increase the efficiency and offset the penalty associated with capturing CO_2 from power generation from fossil fuels. Although these innovative energy systems have significant potential advantages, practical development is hindered by uncertain component performance, the need for new materials, or simply the cost of development. The goal of IEC is to utilize validated, computational simulations that can predict performance of these process technologies to identify gaps in simulations and technology and guide development and accelerate the deployment of IEC technologies.

- **Power Cycling Alternatives** such as power electronics and energetic materials research with application for grid scale energy storage devices to improve reliability and stability of the grid; provide capacity to "peak shave or load shift," enabling peak loads to be met during periods when generation, transmission, and distribution assets cannot yet be brought online; enable the integration of large scale renewable energy plants into the grid; and provide more stable and efficient delivery of electrical power—including power generated from fossil fuel sources. This will result in more stable and efficient delivery of electrical power, while reducing overall CO_2 emissions.

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

Performer: University of Washington

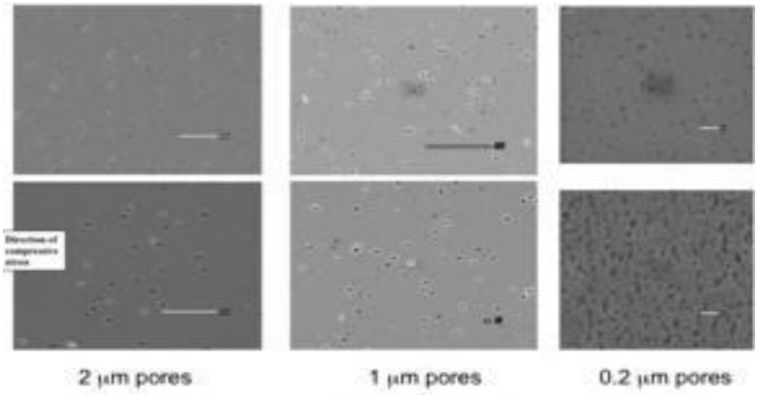
Award Number: FE0007272

Project Duration: 9/21/2011–12/20/2014

Total Project Value: $299,956

Technology Area: University Training and Research

NETL partnered with the University of Washington to explore a novel class of 'n' type thermoelectric oxides that are stable at high temperature in the coal-fired flue gas environment. It will focus on thermoelectric oxides with high figures of merit, employing the recent observation in the literature that thermoelectric figure of merit increases rapidly in the vicinity of the Curie temperature for ferroelectric materials (thermoelectric-ferroelectric coupling). The specific objectives are: (1) to use combinatorial materials exploration to rapidly screen a broad composition range in order to identify the most promising compositions of ferroelectric materials with high Curie temperatures; (2) to investigate the thermoelectric properties of the most promising 'n' type thermoelectric oxides in these families; (3) to develop processing approaches to make oriented crystalline oxides (in order to exploit the expected anisotropic nature of the materials); and (4) to develop processing approaches to make hierarchical anisotropic porous structures in order to evaluate the effect of micro- and macro-pores on thermoelectric properties.This project's success will pave the way for the development of efficient high-temperature, stable thermoelectric modules for waste heat recovery from coal-fired power plants and other industrial systems where process heat is an important byproduct (e.g., steel plants), resulting in higher efficiencies and reduced pollution and greenhouse gases. Another important outcome is the training and education of a PhD student who will work on the scientific issues outlined in the research and will also be exposed to the broader context of research in this important area of energy efficiency and security.



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

Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage

Performer: University of Tennessee, Knoxville

Collaborator(s): University of Tennessee Space Institute

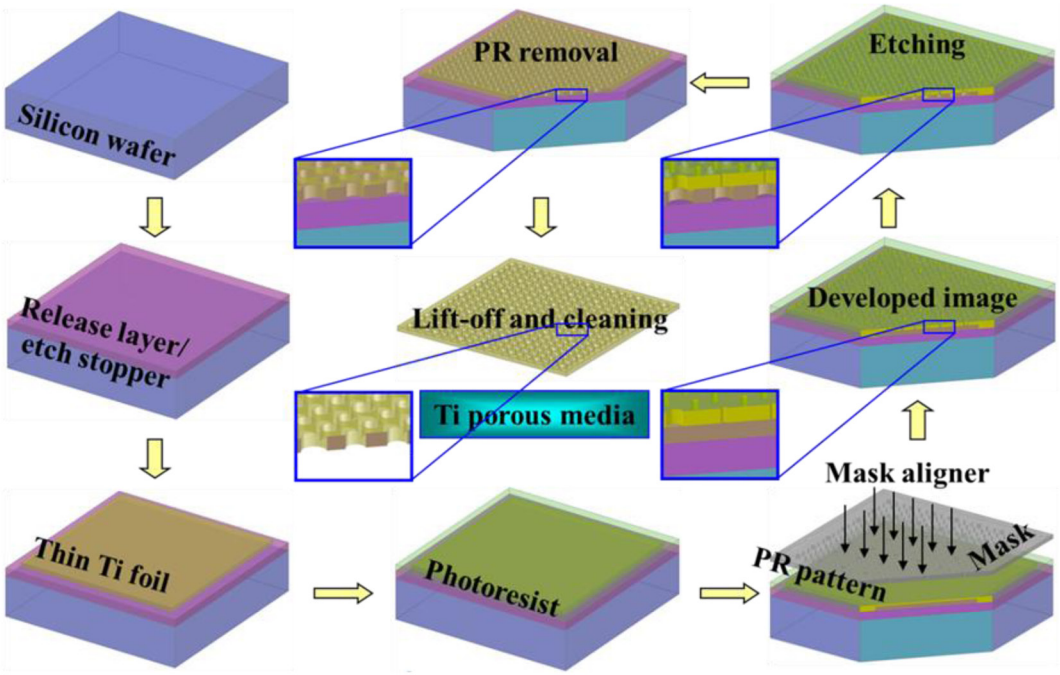
Award Number: FE0011585

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

Total Project Value: $470,084

Technology Area: University Training and Research

NETL is partnering with University of Tennessee to develop thin and well-tunable multifunctional materials of liquid/gas diffusion layers with micro/nano fabrication for high-efficiency electrical energy storage, which is critical for long-term coal energy applications to provide reliable, affordable electricity, and to enable electrical grid modernization. Project goals will be accomplished with theoretical modeling, a fabrication study with thin titanium foils, titanium liquid/gas diffusion layer transport enhancement and surface treatment, and comprehensive *ex-situ/in-situ* characterizations and tests, including the electrolyzer tests of performance and efficiency and 500-hour durability. The successful development will make much thinner and more controllable multifunctional materials with lower flow/interfacial resistances and higher thermal/electric conductivities, thus significantly improving efficiencies of the electrolyzer or other associated energy storage devices.



Fabrication of Ti LGDLs from thin Ti films.

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

Performer: University of Idaho

Award Number: FE0022988

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

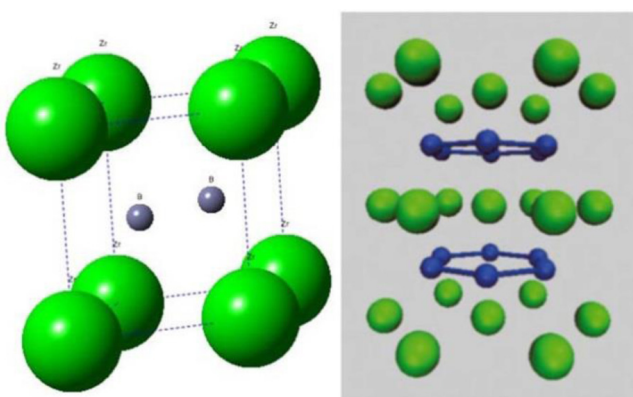
Total Project Value: $399,938

Technology Area: University Training and Research

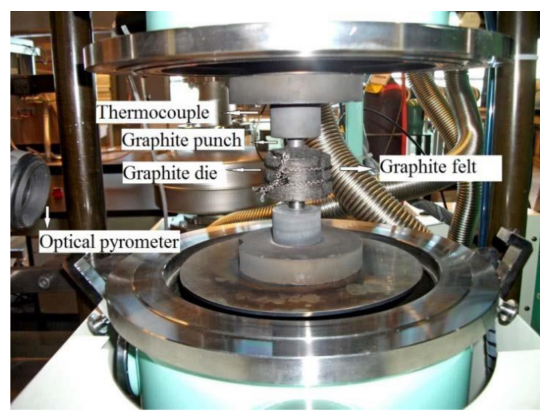
NETL is partnering with the University of Idaho to develop a boride-based ultrahigh temperature ceramic material that possesses all the required properties to function as sustainable electrodes in direct power extraction applications based on magneto-hydrodynamics (MHD). Transition metal borides display 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 will 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 will 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.



Above (left) Hexagonal crystal structure of ZrB_2 and HfB_2 with a symmetry group P6/mmm; (right) Layered atomic arrangement of the diboride structures illustration.



Dr. Sinter 515S machine.

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

Performer: University of Nebraska

Award Number: FE0023061

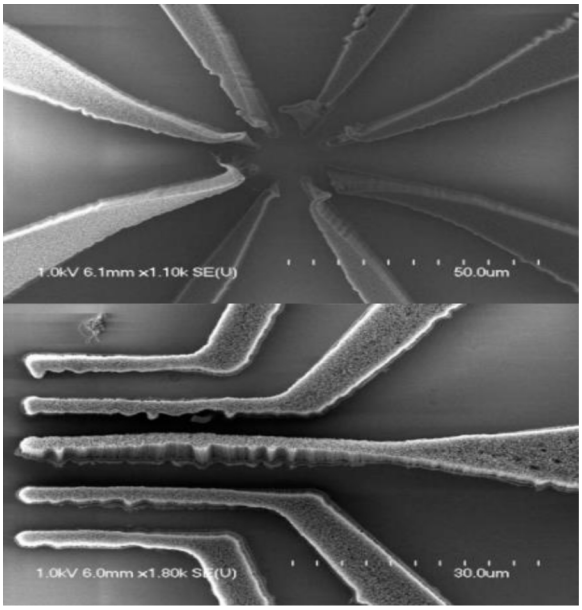
Project Duration: 10/1/2014 – 9/30/2017

Total Project Value: $400,000

Technology Area: University Training and Research

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

The project will provide appropriate composite structures for hot electrode applications without integrating all extreme properties within a single material, stimulate the extensive applications and commercialization of MHD power systems, reduce the capital costs of MHD power systems, establish a new family of VA-CNT-based anisotropic composite structures, and improve electricity generation efficiency in current combustion power plants.



Vertically aligned CNT patterns.

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

Performer: University of Washington

Award Number: FE0023142

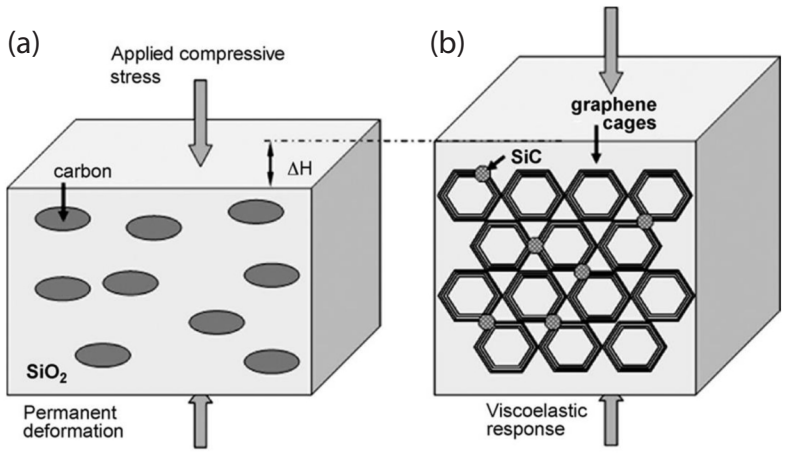
Project Duration: 10/1/2014 – 9/30/2017

Total Project Value: $399,989

Technology Area: University Training and Research

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

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



Two potential models of the carbon dispersion within the SiC bulk material: (a) isolated carbon clusters embedded in the remaining phase; (b) graphene cages encapsulating the remaining phase.

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

Performer: West Virginia University Research Corporation

Award Number: FE0024009

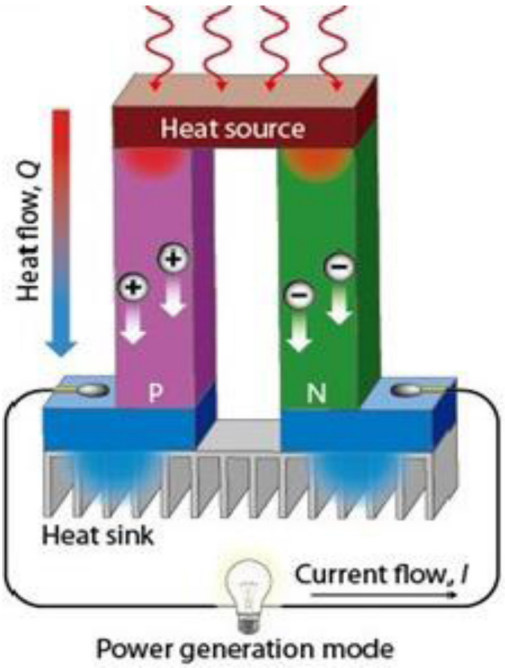
Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $627,160

Technology Area: Plant Optimization Technologies

NETL is partnering with West Virginia University Research Corporation to develop all-oxide thermoelectric generators, which will be highly efficient, cheaply produced, small, lightweight, non-toxic, and highly stable in air at high temperatures, for recovering the waste heat from power systems including solid oxide fuel cells (SOFCs) at temperatures of 600-980 degrees Celsius °C). This project will develop compact and highly efficient all-oxide ceramic thermoelectric generators to work as compact heat exchangers and simultaneously recover the high-temperature waste heat from high-temperature power systems such as SOFCs.

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. Overall, 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 the sensors at temperatures in the 600-980 °C 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.



Thermoelectric Unicouple.

High Temperature High Velocity Direct Power Extraction Using an Open Cycle Oxy Combustion System

Performer: University of Texas at El Paso

Award Number: FE0024062

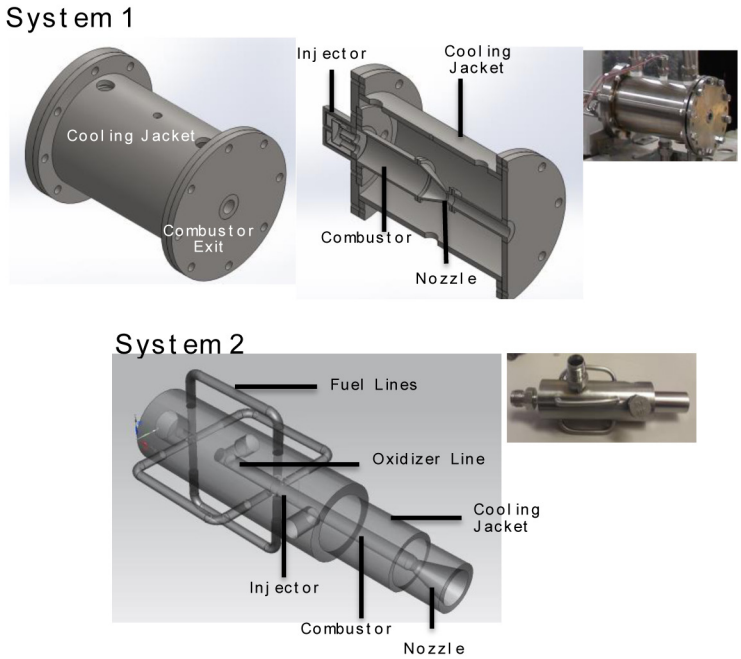
Project Duration: 10/1/2014 – 9/30/2016

Total Project Value: $625,000

Technology Area: University Training and Research

NETL is partnering with the University of Texas at El Paso to develop high-temperature, high-velocity direct power extraction using an open-cycle oxy-combustion system. University researchers will design, optimize, and test a lab-scale high-velocity and high-temperature oxy-fuel combustor, nozzle, and injector for use in direct power extraction magnetohydrodynamic (MHD) applications. To meet this goal, existing facilities will be modified to accommodate a high-temperature and high-velocity oxy-fuel flow. Deliverables include the design, fabrication, characterization, testing, and documentation of the combustor system performance for future use in computational and system development construction of such systems.

The effort will demonstrate the feasibility of MHD oxy-combustion system components for use in electrical power generation, and support the development of energy-efficient technologies that can be used in conjunction with carbon capture techniques. In addition, the outcome of the project will not only improve the fundamental understanding of oxy-fuel combustion and flame stability but also provide critical experimental data for the validation of modeling tools.



High Velocity Thermal Spray equipment to be modified for MHD combustion testing.

Innovative Process Technologies (Task4: Innovative Energy Concepts)

Performer: National Energy Technology Laboratory - ORD

Collaborator(s): Penn State University, West Virginia University, Oregon State University

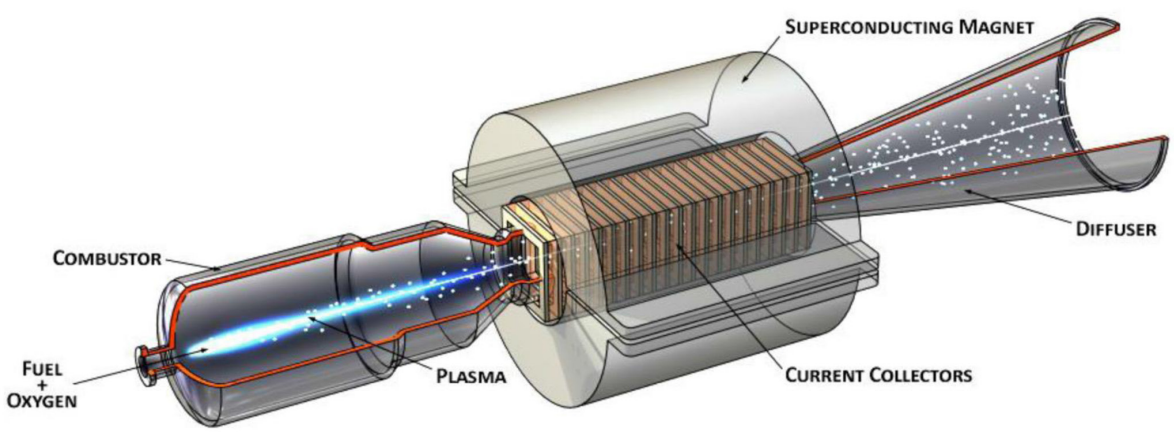
Award Number: FWP-2012.04.01.4

Project Duration: 10/1/2011 – 9/30/2014

Total Project Value: $431,975

Funding Source: Innovative Process Technologies

NETL investigated technologies which could offer a "step-change" in power generation efficiency. NETL focused on direct power extraction (DPE) via magnetohydrodynamic (MHD) principles and on using a rotating detonation engine instead of combustion to drive a gas turbine. The Figure below shows the concept of using oxy-fuel to achieve DPE. The high temperatures possible through oxy-fuel combustion allows for ionization of fuel additives ("seed") and so a high velocity electrical conductive flow can be achieved. By passing such a flow through a magnet, electrical power can be extracted without any mechanical parts. The exhaust gasses can then go to powering a standard bottoming cycle (e.g. steam plant). NETL primarily focused on simulation to better understand and predict performance of these innovative energy systems. Models were built for detonation, high temperature combustion, ionization, and for predicting MHD interactions. In this work, NETL researchers combined and extended several solvers which are distributed with the OpenFOAM library. The project also initiated experimental work with a focus on translational R&D. A particular interest with respect to system performance is quantifying the allowable electrical stresses and current densities within a MHD generator, which is dependent on the channel materials. Low or zero recycle oxy-fuel has the advantage of high temperatures and smaller device sizes, provided material limitations can be quantified and systems developed to fully utilize this advantage. An experiment focused on exposing test samples to the relevant temperatures and electromagnetic fields expected within a MHD channel was developed. Exposure testing will be realized using a high velocity kerosene-oxygen combustor capable of producing 3300 K combustion temperatures and exit velocities of Mach 1.8. A powder injection port allows for introduction of seed. A 2 Tesla electromagnet was selected to provide the necessary magnetic field. Equipment was purchased, and lab set-up activity is underway in FY15 for these tests. Equipment was purchased, and lab set-up activity is underway in FY15 for these tests.



Direct Power Extraction with oxy-fuel.

Abbreviations

C3M ..... Carbonaceous Chemistry for Computational Modeling

COE ..... cost of electricity

CCSI ..... Carbon Capture Simulation Initiative

CO2 ..... carbon dioxide

DOE ..... Department of Energy

EPA ..... Environmental Protection Agency

HBCU/OMI ..... Historically Black Colleges and Universities and Other Minority Institutions (NETL program)

IEC ..... Innovative Energy Concepts

K ..... Kelvin

MHD ..... magnetohydrodynamics

NETL ..... National Energy Technology Lab

NRAP ..... National Risk Assessment Partnership

ORD ..... Office of Research and Development

RAM ..... reliability, availability, maintainability

R&D ..... research and development

SBIR ..... Small Business Innovation Research

SCC ..... Strategic Center for Coal

SiC ..... silicon carbide

UCR ..... University Coal Research (NETL program)

UTR ..... University Training and Research (NETL program)

U.S. ..... United States

UW ..... University of Washington

Contacts

Dr. Robert Romanosky
Acting Technology Manager
Crosscutting Technology Research Program
304-285-4216
Robert.Romanosky@netl.doe.gov

Patricia Rawls
Division Director
Crosscutting Research Division
412-386-5882
Patricia.Rawls@netl.doe.gov

Website: http://www.netl.doe.gov/research/coal/crosscutting/innovative-energy-concepts

Acknowledgements

The Innovative Energy Concepts Portfolio was developed with the support of many individuals. Principal Investigators, Federal Project Managers, Technology Managers, Division Directors, and National Energy Technology Laboratory site-support contractors involved with the preparation of Innovative Energy Concept Portfolio played key roles.

the ENERGY lab

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

420 L Street, Suite 305
Anchorage, AK 99501
907-271-3618

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

13131 Dairy Ashford Road, Suite 225
Sugar Land, TX 77478
281-494-2516

WEBSITE: **www.netl.doe.gov**

CUSTOMER SERVICE: **1-800-553-7681**

U.S. DEPARTMENT OF ENERGY

April 2015