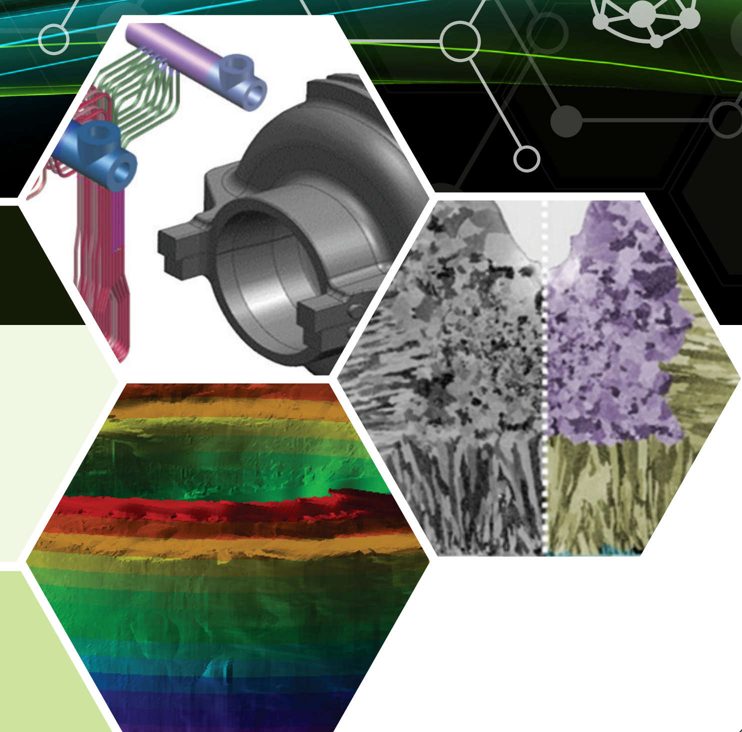
CROSSCUTTING RESEARCH

2022

HIGH PERFORMANCE MATERIALS



PROJECT PORTFOLIO

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

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CROSSCUTTING RESEARCH

NETL's Crosscutting Research Program matures novel technologies that can enhance the efficient performance and eliminate or reduce the environmental impacts of fossil energy power plants. On behalf of the U.S. Department of Energy's Office of Fossil Energy and Carbon Management (FECM), NETL pursues crosscutting research and development (R&D) by collaborating with other government agencies, world-renowned national labs, entrepreneurs, industry, and academic institutions. Efforts are focused on five primary research areas: High Performance Materials; Sensors, Controls, and Novel Concepts; Simulation-Based Engineering; Energy Storage; and University Training and Research (UTR).

The goals are to create transformational technologies under a single research umbrella that improve plant efficiency, flexibility, and security; reduce water consumption; reduce costs; and better enable dependable fossil power systems to maintain the stability and resilience of the electricity grid while maximizing use of variable renewable power sources. The research is leading to enhancements to the fleet such as new ways to address the challenges of load following, better ways to counter cyber intrusions, and advancements in affordable, scalable technical solutions. Because of the broad scope of the Crosscutting Research Portfolio, its technologies often have applicability to other energy-related sectors such as renewable and nuclear power generation, oil and natural gas infrastructure, and aviation (both commercial and military).

Crosscutting Research efforts include sponsorship of two long-running university training programs that prepare the next generation of scientists and engineers to meet future energy challenges. These are the University Coal Research (UCR) program and the Historically Black Colleges and Universities and Other Minority Institutions (HBCU-OMI) program. By working with students on the university level, the efforts ensure that key technologies in areas including advanced manufacturing, cybersecurity, smart data analytics, and high-performance computing will be integrated into fossil plants of the future.

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

High Performance Materials: The High Performance Materials program drives to characterize, produce, and certify cost-effective alloys and other high-performance materials suitable for the extreme environments found in fossil-based power-generation systems. NETL supports and catalyzes a robust domestic materials supply chain that prepares materials for advanced ultra-supercritical (AUSC) steam cycles and spinoff applications. The work also enables research in suitable materials for supercritical carbon dioxide (sCO_2) cycles that yield higher thermal efficiencies.

The Crosscutting Materials program works to accelerate the development of improved steels, superalloys, and other advanced alloys to address challenges of both the existing fleet and future power systems. Materials of interest are those that enable components and equipment to perform in the high-temperature, high-pressure, corrosive environments of an advanced energy system with specific emphasis on durability, availability, and cost both within and across each of four primary platforms: Advanced Manufacturing, Advanced Structural Materials for Harsh Environments, Computational Materials Design, and Functional Materials for Process Performance Improvements.

Sensors, Controls, and Novel Concepts: The Sensors, Controls, and Novel Concepts program is conducting research and development for technologies that will provide pivotal insights into optimizing performance, reliability, and availability of integrated energy and carbon management systems. NETL develops, tests, and matures novel sensor and control technologies that are operable in next-generation energy systems, including hybrid plants incorporating components such as hydrogen-powered turbines and fuel cells, renewables, and energy storage applications. These sensors enable responsiveness to varying conditions in real time, maintaining high efficiencies and reducing emissions.

The Crosscutting Sensors, Controls, and Novel Concepts program explores advances within and the integration of technologies across the following primary research areas: Harsh Environment Sensors, Advanced Controls and Cyber Physical Systems, and Novel Concepts.

Simulation-Based Engineering: Simulation-Based Engineering (SBE) focuses on developing and applying advanced computational tools at multiple scales: atomistic, device, process, grid, and market scales, to accelerate development and deployment of fossil fuel technologies. Research in this area provides the basis for the simulation of engineered devices and systems to better predict and optimize the performance of fossil fuel power generating systems.

Computational design methods and concepts are required to significantly improve performance, reduce the costs of existing fossil energy power systems, and enable the development of new systems and capabilities such as advanced ultrasupercritical combustion and hydrogen turbines.

This effort combines theory, computational modeling, advanced optimization, experiments, and industrial input to simulate complex advanced energy processes, resulting in virtual prototyping. The research conducted in the SBE R&D develops accurate and timely computational models of complex reacting flows and components relevant to advanced power systems. Model development and refinement is achieved through in-house research and partnerships to utilize expertise throughout the country.

Energy Storage: Energy Storage aims to develop a comprehensive strategy to expand FECM's current portfolio of technologies and programs in order to better enable fossil power plants to maintain the electricity grid's stability and resilience while increasingly utilizing variable renewable power. Energy storage at the generation site will be essential to a resilient and flexible electricity network and NETL's Energy Storage program aims to address the needs and challenges of site storage. The goal of this program is to leverage over a century of investment in fossil energy infrastructure, extend the useful lifetime of existing fossil energy assets, enhance the role of fossil assets as contributors to grid stability and reliability, and provide the nation with a reliable fossil-based option by leveraging and extending ongoing energy storage technology development.

University Training and Research: University Training and Research supports two of the longest-running university training programs, the Historically Black Colleges and Universities and Other Minority Institutions (HBCU-OMI) and the University Coal Research (UCR) programs, to support the education of students in the area of carbon management. Both programs are promoted through research grants to U.S. colleges and universities that emphasize FECM strategic goals. These training programs were designed to increase the competitiveness of universities in fossil energy research and discoveries. The student-led research programs advance energy technologies and allow for expansion of energy production while simultaneously facilitating energy sector job growth.

HIGH PERFORMANCE MATERIALS

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

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

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

- Advanced Manufacturing
- Advanced Structural Materials for Harsh Environments
- Computational Materials Design
- Hydrogen Production

Specific Technology Objectives:

- Develop computational materials modeling to enable rapid design and simulation of new and novel alloy materials. Computational design of materials has the potential to produce major breakthroughs.
- Develop superalloys and ferritic materials for use in AUSC conditions of 760 degrees Celsius (°C) and 350 bar pressure (5,000 psi) to reduce costs, improve corrosion and erosion resistance, increase material strength, and reduce wall thickness.
- Develop functional materials for energy storage and high-performance materials with mechanical properties that can perform reliably at temperatures well over 1,000 °C.
- Develop advanced metallic and ceramic coatings, including nanomaterials, to provide thermal barrier protection for turbine blades, combustor components, and tubing.
- Develop validated computational models capable of simulating and predicting performance of materials in various types of transformational power plants.

This project portfolio report showcases 33 high-performance materials projects within the Crosscutting Research Program of the Technology Development Center. Each of the pages reporting on projects describes the technology, the program goals, and overall benefits.

ADVANCED MANUFACTURING

Standardized Test Method and Calculation Protocol for Determining and Reporting Annual Heat Rate for Coal-Fueled Electricity Generating Units

Performer	**ASME Standards Technology, LLC**
Award Number	FE0031933
Project Duration	09/26/2020 – 03/31/2022
Total Project Value	$ 382,451
Technology Area	Plant Optimization Technologies

The objective of this effort is to establish an industry-acceptable standard heat rate test method and annual/long-term heat rate calculation protocol for coal-fired electricity generating units. This study will cover two areas of primary concern related to the development of methodologies to publish The American Society of Mechanical Engineers (ASME) Standards to provide regulators and industry with procedure(s) to report annual heat rates.

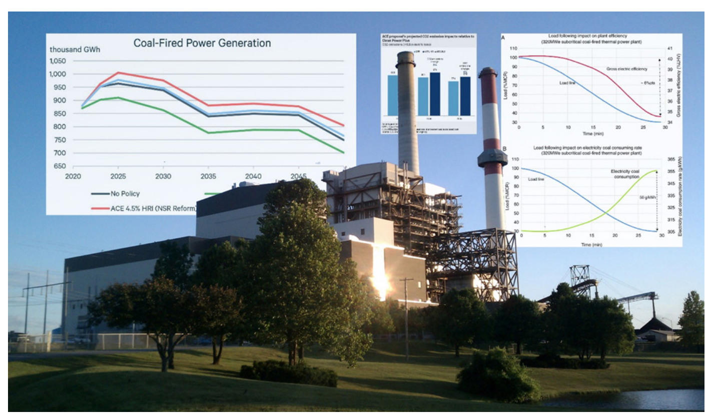
The first area is to survey government agencies, utilities, and non-government organizations who have primary interest in regulating or producing electric power from coal-fired plants. This will include their concerns regarding reporting of heat rate data and issues of data accuracy.

The second major area will be to use the existing ASME Codes and Standards procedures to provide a consensus methodology to report annual/long-term heat rates for coal-fired power plants. ASME Performance Test Codes provide procedures that yield results of the highest level of accuracy consistent with the best engineering knowledge and practice currently available. The ASME Code will be developed by balanced committees representing all concerned interests and will specify procedures, instrumentation, equipment-operating requirements, calculation methods, and uncertainty analysis.

Heat rate improvements are an economical and proven method to reduce fuel usage and overall plant emissions, including CO_2. In order to assess if changes to operating procedures or equipment installation are beneficial in improving heat rate, an accepted calculation and reporting protocol is required to establish a baseline that industry and government can observe and utilize for decision making. Reported heat rates are an important tool used by industry and regulators:

- An important consideration for power plant dispatch
- Indicator of reduced fuel use and improved operating economics
- Emissions assessment and reduction (e.g., CO_2)
- Monitor plant performance and assist in analysis of impact cycling and startup/shutdown operations

This effort will establish such a standard and protocol for coal-fired electricity generating units.



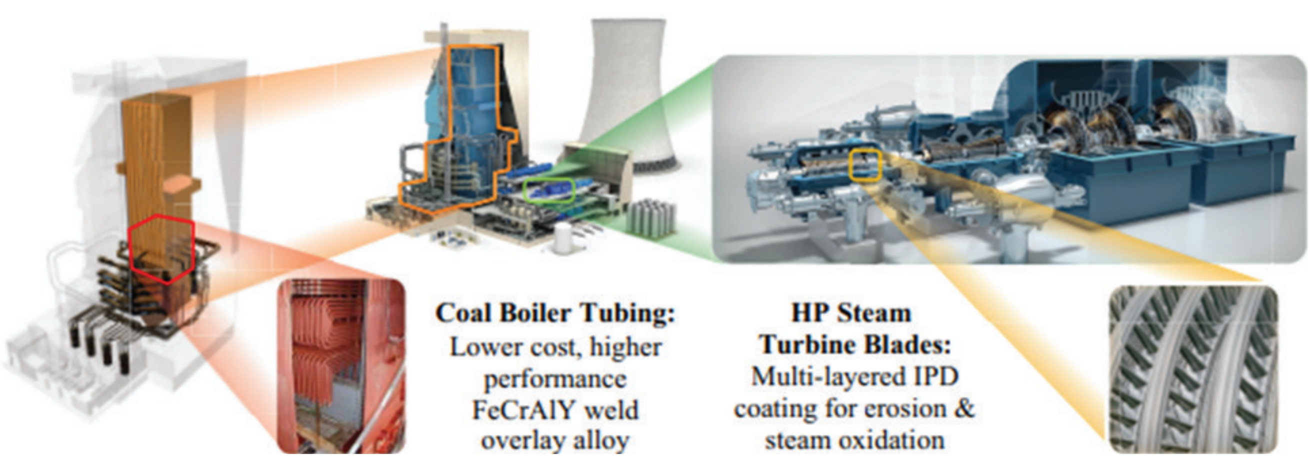
Advanced Coating Compositions and Microstructures to Improve Uptime and Operational Flexibility in Cyclic, Low-Load Fossil Plants

Performer	**General Electric (GE) Company**
Award Number	FE0031911
Project Duration	09/01/2020 – 08/31/2023
Total Project Value	$ 5,549,995
Technology Area	Plant Optimization Technologies

This project addresses two principal factors that drive outages in the fossil power plant fleet: corrosion at the outer diameter of boiler tubing and solid particle erosion in high-pressure (HP) steam turbine blades. The overarching objective is to produce coatings that mitigate these damage mechanisms and provide a comprehensive solution to improve fleet reliability and operational flexibility. GE Research will lead a team of researchers to leverage a century of fleet experience and exciting new results obtained from DOE-funded nuclear materials research to develop cost-effective weld overlay compositions for boiler tubing and multi-layered ion plasma deposition coatings that deliver improvements in both erosion and oxidation resistance in high temperature steam for HP turbine blades. Deep technical expertise and world class characterization capability will be provided by Oak Ridge National Laboratory and the University of Tennessee. The team will work collaboratively through a robust, logical project map to achieve the objectives listed below, identified based on the funding announcement and direct input from GE:

- Enable a 25%-50% increase in time between outages for both boilers and HP turbines.
- Eliminate or significantly reduce the nickel content in weld overlay to mitigate cost.
- Provide adequate oxidation resistance for HP turbine inlet steam at >620 °C and >220 bar.
- Apply coatings to actual components, using today's production-scale methods.

Decreased component cost, increased performance, and extended time between outages are direct value propositions for the fossil energy fleet. For the U.S consumer, project success could lead to increased grid reliability (fewer unexpected outages), decreased levelized cost of electricity, and reduced environmental impact due to low-loading/load following to accelerate penetration of renewables.

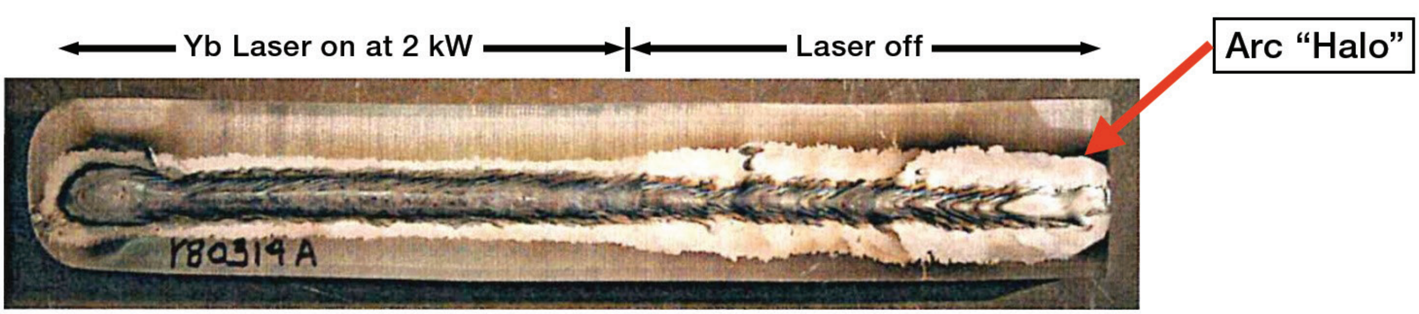


Multi-pass Hybrid Laser Arc Welding of Alloy 740H

Performer	**Idaho National Laboratory (INL)**
Award Number	FWP-B100-19010
Project Duration	10/01/2019 – 09/30/2022
Total Project Value	$ 1,294,000
Technology Area	Plant Optimization Technologies

Idaho National Laboratory will employ hybrid laser arc welding techniques to initially weld thick weld groove land areas (approximately 0.5" thick) using deep laser penetration tactics that, among other features, incorporate a laser wobble head to stabilize the “keyhole” region of the laser weld. Subsequently, the remaining narrow weld groove will be rapidly filled with filler metal using hybrid laser arc welding. The laser wobble head will also be used in this step to improve sidewall tie-in and reduce welding defects, resulting in an overall improvement to the weld strength reduction factor. Finally, the project team will make a complete weld in 3”-thick plate Inconel alloy 740H. Total welding time will be compared with conventional welding practices and welds will be characterized for microstructure and mechanical properties, including long-term (approximately 10,000 hours) creep testing.

This work seeks to reduce the time it takes to weld thick sections of Inconel 740H by up to a factor of two and improve weld quality. This project could provide a foundation for the acceptance of hybrid laser arc welding as a high-productivity joining method, reducing overall construction costs and construction time.



The benefits of laser stabilization in hybrid laser arc welding on Inconel 740H.

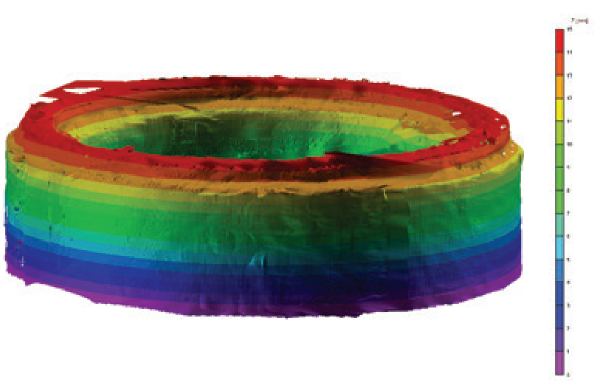
Development of Functionally Graded Transition Joints to Enable Dissimilar Metal Welds

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA151
Project Duration	07/01/2019 – 09/30/2022
Total Project Value	$ 1,000,000
Technology Area	Plant Optimization Technologies

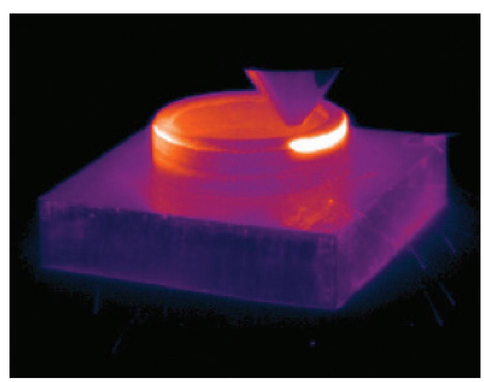
Oak Ridge National Laboratory will weld dissimilar metals using functionally graded transition joints that exhibit high resistance to creep and fatigue and high microstructural stability. The primary focus of the project will be on joining ferritic steels to austenitic steels, in particular alloys that are relevant in coal-fired power plants. A key aspect of the R&D activities will be determining optimum compositional profiles of the transition joint, which will be achieved using computational materials science and engineering. Another key aspect will be avoiding sharp changes in the carbon chemical potential of the joint region. The project entails the integration of several interrelated tasks to achieve project objectives.

- Design optimization of chemistry/microstructure transitions in graded transition joints to minimize carbon diffusion and the formation of stresses induced by thermal expansion mismatch.
- Optimization of processing methods to fabricate the graded transition joint and in situ process monitoring to qualify components. The effect of using powders or wires as feedstock on manufacturability and costs will be addressed, as well as practical aspects of deploying the technology to the field.
- Evaluation of mechanical performance of the transition joints using ex situ and in situ testing as a function of processing parameters, and comparison with historic creep rupture properties of dissimilar metal welds.

The successful completion of this project will set the stage for subsequently developing an ASME code case for wide industrial acceptance and utilization of this technology.



In-situ Imaging of joint during fabrication. Color corresponds to vertical height.

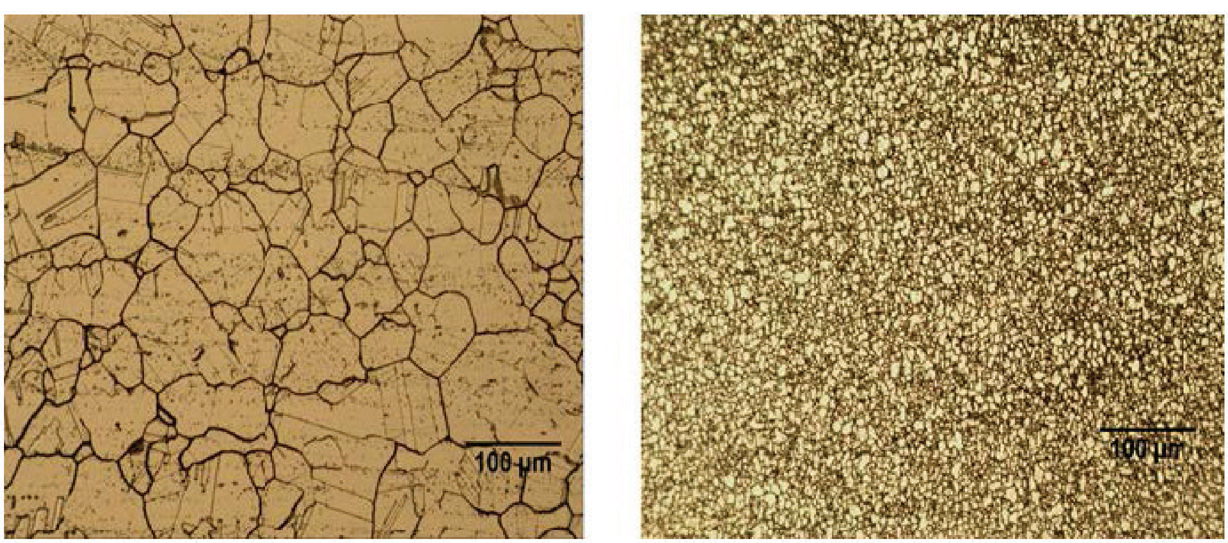


IR image showing temperature distribution with build height.

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

Performer	**Pacific Northwest National Laboratory (PNNL)**
Award Number	FWP-71843
Project Duration	10/01/2018 – 06/30/2022
Total Project Value	$ 1,120,000
Technology Area	Plant Optimization Technologies

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



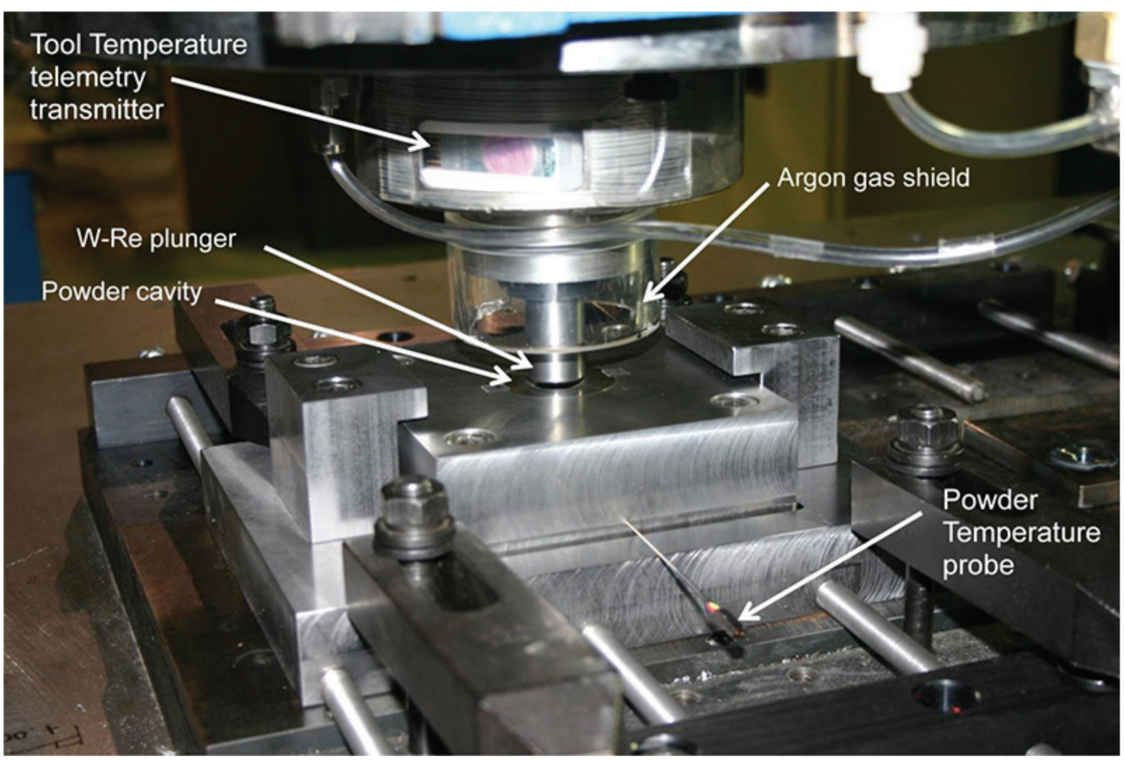
Haynes 282 microstructure comparison of base material (left) and FSW weld nugget (right).

Low Cost Fabrication of ODS Materials

Performer	**Pacific Northwest National Laboratory (PNNL)**
Award Number	FWP-60098
Project Duration	10/01/2010 – 09/30/2022
Total Project Value	$ 735,000
Technology Area	Plant Optimization Technologies

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

The project will contribute to more efficient use of fossil fuels in advanced ultrasupercritical power plants, which will concurrently lead to reduced discharge of carbon dioxide and other emissions.



Friction extrusion die at Pacific Northwest National Laboratory.

Solid State Joining of Creep Enhanced Ferritic Steels

Performer	**Pacific Northwest National Laboratory (PNNL)**
Award Number	FWP-66059
Project Duration	10/1/2014 – 06/30/2022
Total Project Value	$ 1,075,000
Technology Area	Plant Optimization Technologies

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

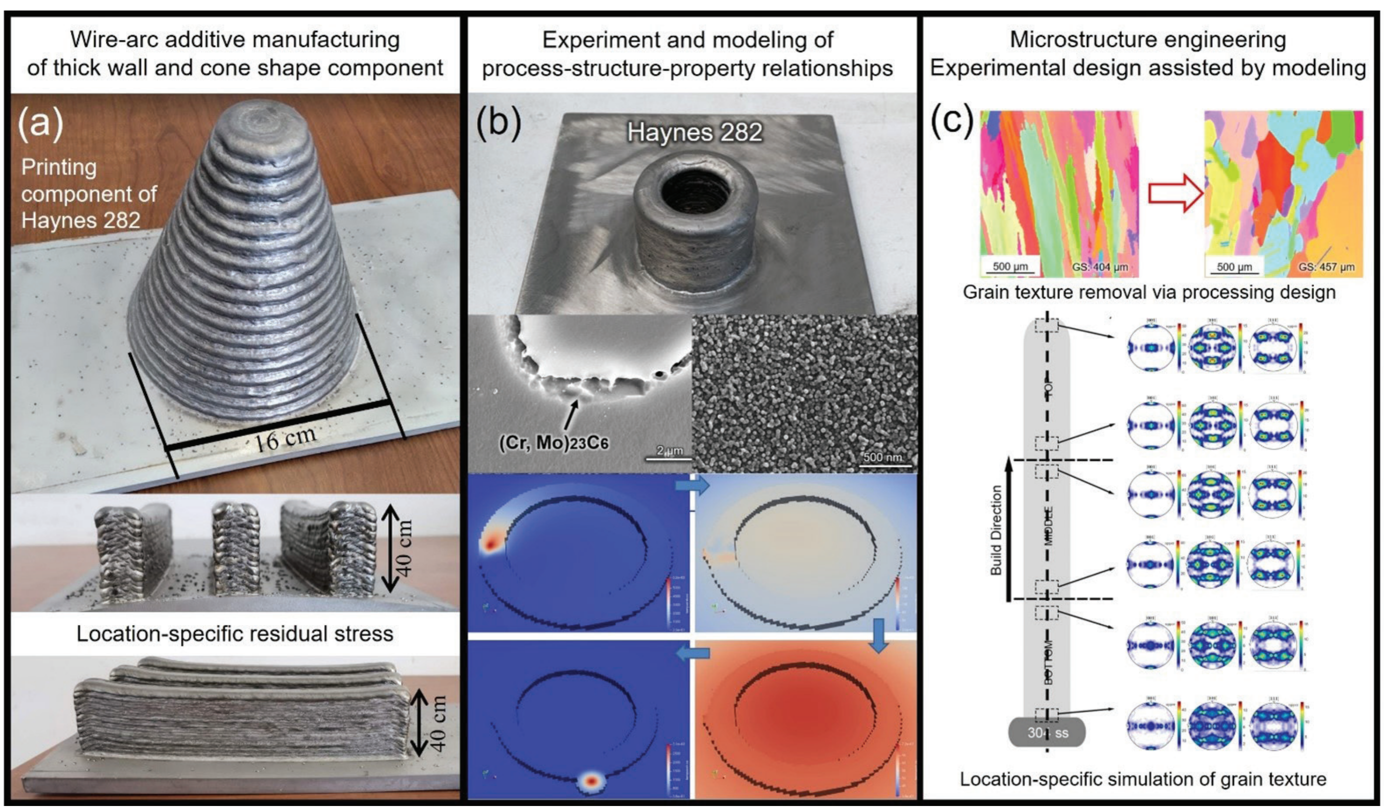
It is expected that higher performance CSEF steels used in AUSC coal-fired power plants will improve efficiency and operational flexibility and result in lower operating costs.

Flat plate friction stir welds in HSLA65 plate.

Wire Arc Additive Manufacturing of Advanced Steam Cycle Components Using Location Specific Design Enhanced by High-Throughput Experiments and Machine Learning

Performer	**University of Pittsburgh**
Award Number	FE0026825-06-19
Project Duration	02/01/2021 – 01/31/2023
Total Project Value	$ 640,225
Technology Area	Plant Optimization Technologies

The research team at the University of Pittsburgh (Pitt) will perform location specific design for Wire Arc Additive Manufacturing (WAAM) of Haynes 282 superalloys through the extended ICME (Integrated Computational Materials Engineering) platform with further enhancement by machine learning (ML) and high throughput experiments on process-structure-property relationships. The location-specific ICME design will significantly improve the overall quality of thick wall (> 1 inch) components with complex shape fabricated by WAAM. This project could enable applying the WAAM technology to fabricate or repair advanced steam cycle components with desirable strengths at elevated temperatures for the efficient operation of advanced fossil energy power plants. An extended ICME design framework for WAAM of part scale components will be delivered through this project and can be readily extended to other high-performance alloys.

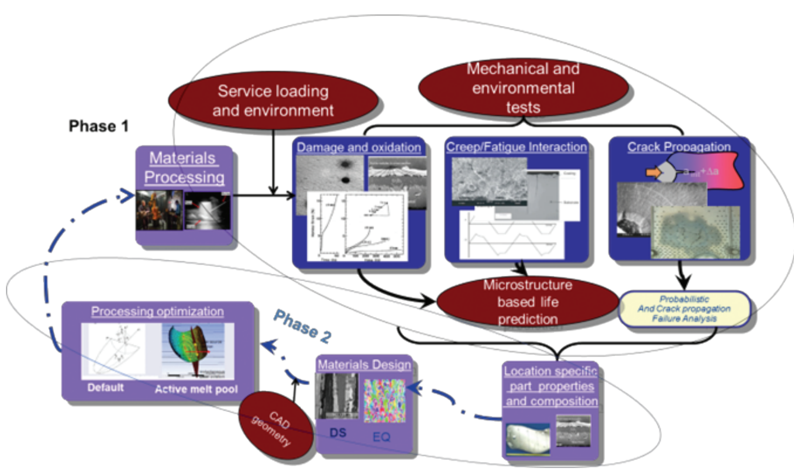


Optimization of Wire Arc Additive Manufacturing (WAAM) Process to Produce Advanced Ultra-Supercritical Components (AUSC) Components with Increased Service Life

Performer	**Raytheon Technologies**
Award Number	FE0031821
Project Duration	10/01/2019 – 02/28/2022
Total Project Value	$ 1,249,916
Collaborator	Siemens
Technology Area	Plant Optimization Technologies

The objective is to develop the capability for large area Wire Arc Additive Manufacturing (WAAM) to produce functionally graded AUSC components with location specific morphology and composition to increase structural life in severe service conditions. The recipient will integrate physics-based material and damage modeling into an additive manufacturing control system to produce and test materials engineered for an aggressive environment, extreme high temperature, and very long operation time regimes.

The project will augment the WAAM process to produce fossil energy system components with tailored properties though functionally graded microstructure. In phase 1, a physics-driven process model will be used to generate a novel build strategy that can produce directionally solidified and equiaxed morphology in the same component while utilizing localized heating, cooling, and modified feedstocks. Raytheon Technologies will study the artificial intelligence and physics-based models for the development of extremely efficient numerical methodology for both production using WAAM and for long-term life prediction. The research team will perform techno-economic analysis based on WAAM process data to understand the cost savings obtained through improved design life due to tailored microstructure and composition. Verification of the models consists of comparison with coupon and feature-test results. Phase 1 will develop the basis of WAAM process augmentation through microstructure control by evaluating the impact of environmental effect and manufacturing processes on materials microstructure and properties through mechanical tests under relevant conditions, estimate the technoeconomic entitlement, and assess candidate valve geometry.



An Integrated Computational Materials Engineering framework connecting process-structure-properties-performance by models.

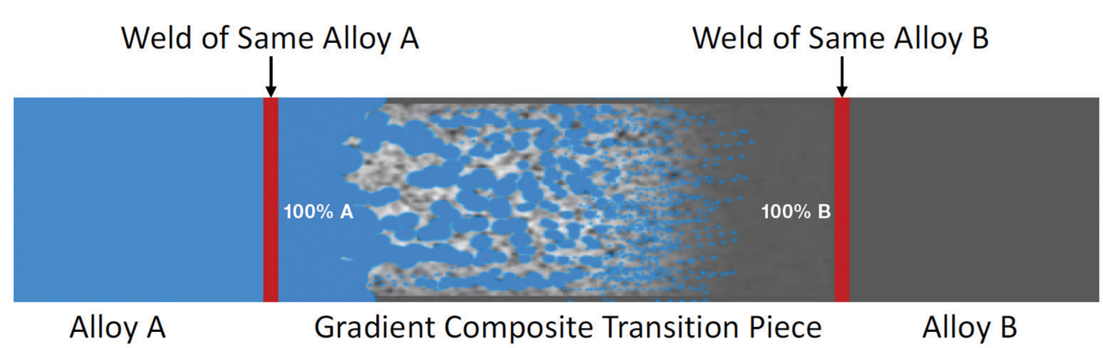
Additively Manufactured Graded Composite Transition Joints for Dissimilar Metal Weldments in Utra-Supercritical Power Plant

Performer	**West Virginia University**	**Oak Ridge National Laboratory (ORNL)**
Award Number	FE0031819	FWP-FEAA372
Project Duration	10/01/2019 – 09/30/2024	10/01/2019 – 09/30/2021
Total Project Value	$ 7,289,004	$ 310,000
Total Project Value (All)	$ 7,599,004	
Collaborators	Carpenter Powder Products; General Electric; Oak Ridge National Laboratory	
Technology Area	Plant Optimization Technologies	

The objective of this project is to develop and demonstrate at lab scale the additively manufactured graded composite transition joints (AM-GCTJ) for dissimilar metal weldments (DMW) in next-generation advanced ultra-supercritical (AUSC) coal-fired power plants, that can significantly improve the microstructural stability, creep, and thermal-mechanical fatigue resistance as compared with their conventional counterparts.

Conventional DMW interfaces of P91/Super 304H and Super 304H/282 will be characterized by neutron diffraction measurement at Oak Ridge National Laboratory (ORNL)'s Spallation Neutron Source (SNS) under simulative thermal cyclic conditions to understand the thermal stresses and establish the baseline. In collaboration with the experimental microstructure characterization and creep and thermal creep fatigue testing tasks, the ORNL's integrated computational weld engineering (ICWE) model framework will be used to simulate the microstructure and property variations and their effects on the thermal stresses in the AM-GCTJ.

The successful completion of this project will develop cost-effective and readily scalable AM-GCTJ that practically eliminates the coefficient of thermal expansion mismatch and sharp compositional transition associated with DMW. The AM-GCTJ will significantly improve the high-temperature mechanical properties as compared with their conventional DMW counterparts. This is not only a key technology advancement toward the development of next generation AUSC plants, but also may extend the lifetime of current fleets that have been through frequent cycling.



Concept of additively manufactured graded transition joint.

Conformal Coatings on Additive Manufactured Robust Alloys for Significant Mitigation of Oxidation, Erosion, and Corrosion

Performer	**West Virginia University Research Corporation**
Award Number	FE0032068
Project Duration	09/15/2021 – 09/14/2024
Total Project Value	$ 400,000
Technology Area	University Training and Research

The project will develop novel high-temperature alloys from nickel (Ni)-based alloys that further integrate additive manufacturing (AM) fabrication, creating novel nanoscale oxide precipitation for strengthened mechanical integrity and enhanced oxidation resistance, and subsequent application of conformal protective coatings on the additive manufactured alloys. To increase the strength and oxidation resistance of nickel alloys, erbium and titanium oxide (Er_2O_3 and TiO) precipitants will be added to the AM powders for the Inconel 625 alloy and result in dense nano-oxide precipitation of Er_2O_3 and $Er_2Ti_2O_7$, which will result in a solution-strengthened novel Ni-based alloy. Furthermore, a conformal protective oxide coating layer will be simultaneously applied on both the internal and external surface of the additive manufactured heat exchangers with complex geometry using atomic layer deposition (ALD). The ALD layer will be conformal, uniform, pin-hole free, dense, and ultra-thin with negligible weight gain to increase both the oxidation and corrosion resistance at elevated temperatures.

The project is organized into 5 Tasks. Task 1 is project management. Task 2 is devoted to introducing the dense precipitates into the Ni-based alloys through AM. Task 3 is devoted to ALD coating of the newly additive manufactured 3D printed Ni-based alloys and ALD repairing and recoating the alloys after oxidation exposure. Task 4 is the oxidation resistance testing of the additive manufactured and ALD coated Ni-based alloys. Task 5 is the comprehensive physical properties testing, and nanostructure analysis of the additive manufactured alloys (including the ones with precipitates), ALD coated alloys, and the alloys after exposure to the oxidation and corrosion environments.

The developed high-temperature materials are expected to possess superior strength, high resistance to external surface oxidation, internal surface carburation, and corrosion, and can be applied to heat exchangers for operation in supercritical carbon dioxide at high temperatures (over 750 °C) and pressure (30 MPa). For after-service heat exchangers that have damaged surfaces, the ALD coating can also be utilized to repair/refurbish the heat exchanger parts that may have been impacted by surface oxidation and dramatically increase their lifetime and reduce costs.

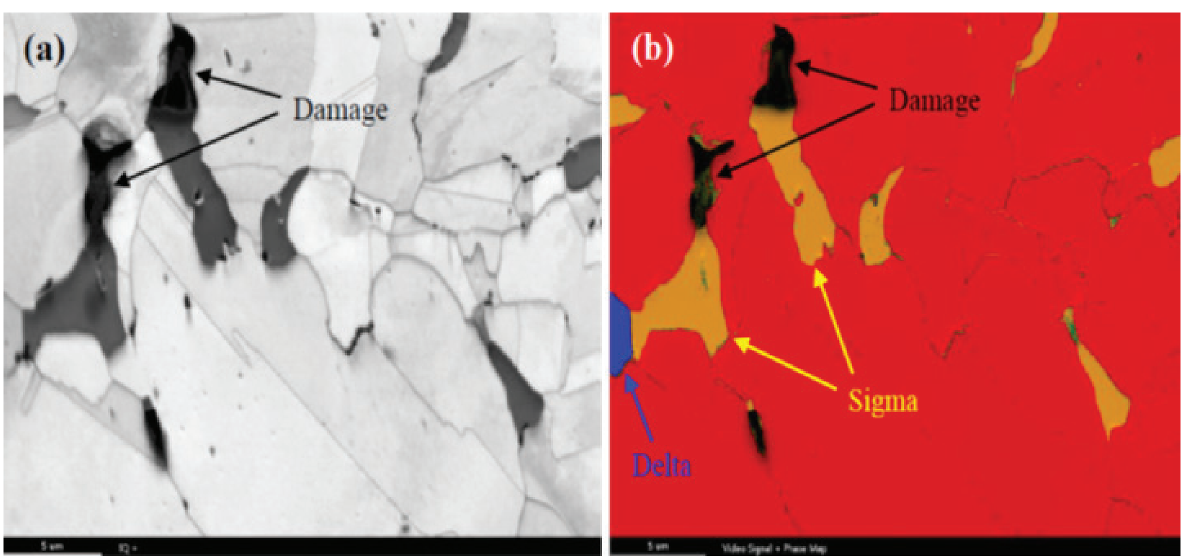
ADVANCED STRUCTURAL MATERIALS FOR HARSH ENVIRONMENTS

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

Performer	**Electric Power Research Institute, Inc.**
Award Number	FE0031562
Project Duration	01/25/2018 – 03/31/2022
Total Project Value	$ 2,800,000
Technology Area	Advanced Combustion Systems

NETL partnered with the Electric Power Research Institute to provide a comprehensive database of mechanical properties, damage assessment/accumulation, and microstructural information from extreme environment material (EEM) components subjected to long-term service with the intent to develop, calibrate, refine, and/or validate the life assessment tools used for predicting remaining life under complex operating conditions. Sufficient quantities of EEM components will be obtained from operating and decommissioned coal-fired power plants. The materials obtained will have been exposed to long-term service (greater than 100,000 hours) and will include all relevant background information for material type, fabrication data, and operational conditions. The acquired materials will be subjected to detailed damage analysis, in-depth microstructural characterization, and, where relevant, rigorous low- and/or high-temperature mechanical testing in an effort to establish a link between microstructural/damage evolution and long-term behavior as established by in-service performance, destructive evaluation, or predicted behavior through time-temperature-parameter relationships or continuum damage mechanics.

The results obtained from this project will provide a comprehensive compendium of materials data and time-temperature-parameter relationships for EEM components exposed to long-term service in coal-fired power plants.



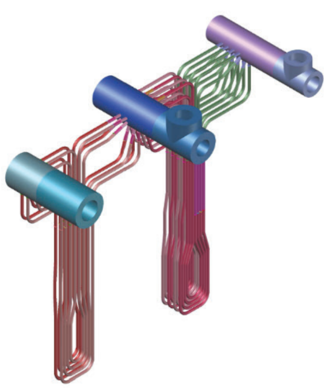
(a) Scanning electron microscope image and (b) corresponding electron backscatter diffraction phase map showing creep damage associated with sigma phase in 374H.

Advanced Ultra-Supercritical Component Testing

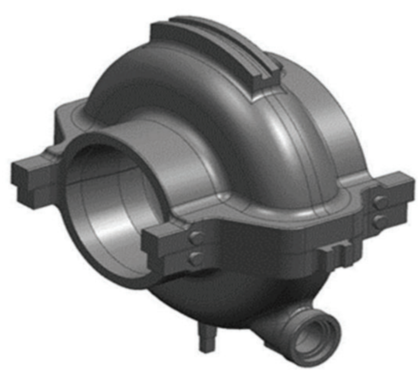
Performer	**Energy Industries of Ohio, Inc.**
Award Number	FE0025064
Project Duration	11/01/2015 – 02/28/2022
Total Project Value	$ 27,311,822
Collaborators	AECOM; Alstom Power, Inc.; Electric Power Research Institute, Inc.; GE Power and Water; MetalTek International; Riley Power; Special Metals; Thermal Engineering; Youngstown Thermal
Technology Area	Plant Optimization Technologies

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

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



AUSC superheater/reheater assembly.



Nozzle carrier casting.

Robust Dissimilar Metal Friction Welded Spool for Enhanced Capability for Steam Power Components

Performer	General Electric (GE) Company
Award Number	FE0031907
Project Duration	09/01/2020 – 08/31/2023
Total Project Value	$ 6,249,846
Technology Area	Plant Optimization Technologies

General Electric Company will undertake a three-year, $6.25 million project to improve the durability of dissimilar metal welds (DMWs) for boiler and heat recovery steam generator (HRSG) applications with reduced maintenance costs and enhanced capability of plant cycling operations. The Recipient will develop a durable friction-welded dissimilar-metal spool utilizing the higher capability transition material of a nanostructured ferritic alloy (NFA) and an oxidation protective coating across weld joints that can be retrofitted to the existing fleet. The spools will be friction-welded in the shop, allowing for controlled friction-welding procedures, post-weld heat treatment, and non-destructive evaluation (NDE). These spools can then be welded with same-metal fusion welds as replacements or upgrades in the field. Improved joint durability will enable at least a fivefold increase in the number of cold starts and reduce unplanned outages from DMW failures.

Improving the durability of the DMW joints reduces the number of unplanned outages and associated maintenance costs. The improved properties of the joint provided by friction welding and an NFA transition piece can enable an increased number of cold starts and more cycling of the boiler and HRSG systems. Preliminary evaluation of a friction-welded spool showed a fivefold increase in the number of cycles before failure of the joint compared to a baseline traditional DMW. This improvement in life and DMW reliability would lead to less unplanned downtime and longer maintenance windows.

Rotary friction welded T91 to 304H tube.

A Novel Surface Technology with a Superalloy Composition as a Low-Cost Solution for Protecting Boiler Tubes Against Failure

Performer	**Maxterial, Inc.**
Award Number	SC0021588
Project Duration	02/22/2021 – 02/21/2022
Total Project Value	$ 206,500
Technology Area	Plant Optimization Technologies

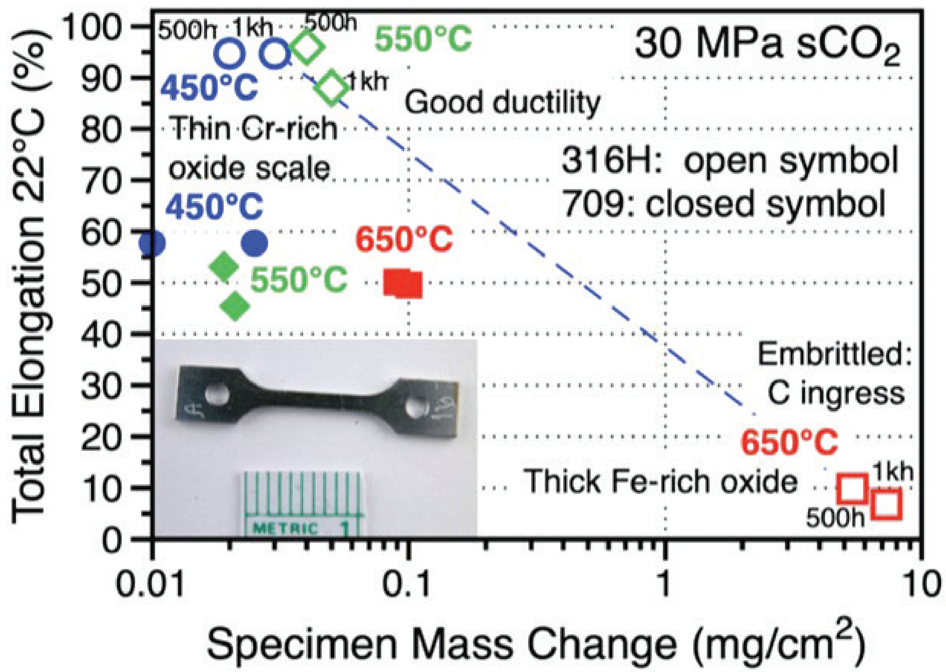
This project will develop a low-cost and highly corrosion-resistant coating for enhancing the resistance of boiler tubes against failure. Protecting boiler tubes against thermal failure is an emergent need in coal power plants. The reason is that many of these boilers are now experiencing on/off cycling operation though they were originally designed for continuous operation. Increasing the corrosion resistance of boiler tubes will result in savings to the power plant due to decreased downtime, fewer repairs, and fewer replacements for boiler tubes.

Effect of Impurities on Supercritical Carbon Dioxide Compatibility

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA144
Project Duration	10/01/2019 – 09/30/2023
Total Project Value	$ 1,650,000
Technology Area	Plant Optimization Technologies

This project will study the effect of impurities (e.g., O_2, H_2O) on compatibility of structural materials in supercritical carbon dioxide (sCO_2) Brayton cycle systems, particularly for direct-fired systems. For economically scaling up to commercial power production, the increased use of Fe-based alloys is needed and impurity studies at (450-650 °C) will determine operating limitations for 9-12% Cr and austenitic steels. In addition to measuring reaction rates and characterizing reaction products, post-exposure room-temperature tensile properties will be used to quantify compatibility as a function of temperature, time, and impurity level. After establishing baseline behavior, coatings and shot peening will be evaluated to increase the maximum temperature capability of Fe-based structural alloys. This information will be used to continue the development of a lifetime model for various classes of structural alloys with and without surface modifications. Previously, high O_2 impurity levels (0.25-1%) have been found to increase reaction rates of both Fe- and Ni-based alloys at 750 °C/300 bar (30 MPa). Further work is needed to isolate O_2 and H_2O effects including the use of isotopic tracers. An additional project goal is to understand creep behavior of thin-walled sections for Fe- and Ni-based alloy heat exchangers.

Supercritical CO_2 (sCO_2) is of increasing interest in a broad range of energy applications, especially for waste heat recovery but also to replace water/steam. If sCO_2 systems could be scaled up from the current <10 MW size this would enable use in power generation in coal, natural gas (bottoming cycle), nuclear (power and propulsion), and concentrated solar power systems. The advantages of sCO_2 are (1) low critical temperature and pressure (31 °C/73.8 bar), (2) single phase over a wide temperature and pressure range, (3) high thermal capacity and density leading to smaller turbomachinery, and (4) low work for recompression (e.g., compared to He). Closed Brayton cycle systems (like sCO_2) operate at higher pressures to increase efficiency, and these higher pressures require new designs for airfoils, seals, and heat exchangers while typically lowering the working fluid temperature significantly compared to combustion turbines. These new designs may necessitate new materials or processing methodologies. Materials are a key concern for the scale-up to commercial size, particularly the use of lower-cost steels where applicable. Recently, unique experimental equipment was developed at ORNL for simulating controlled impurity levels in sCO_2 conditions. Initial testing was conducted at 750 °C/300 bar and found accelerated corrosion rates compared to research-grade sCO_2, particularly for Fe-based alloys. The next phase of this study is examining steels at lower temperatures where they have sufficient strength. The initial results suggest that all of the candidate steels are showing faster corrosion rates with the addition of impurities and the next phase of coating evaluations is needed.

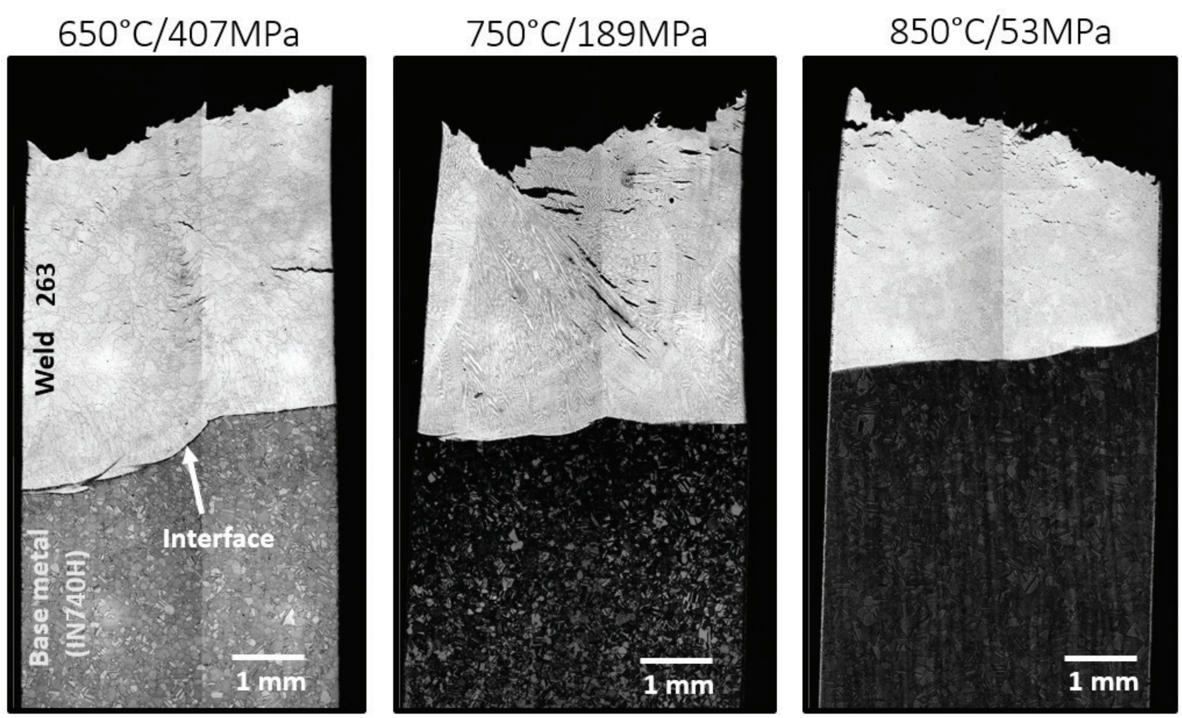


Specimen mass change plotted versus the post-exposure room temperature ductility (total elongation in tension with a strain rate of 0.015/min per ASTM E8-13). The open symbols are for type 316H stainless steel and the closed symbols for alloy 709 with 20Cr-25Ni.

Evaluating Ni-Based Alloys for A-USC Component Manufacturing and Use

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA152
Project Duration	10/01/2019 – 09/30/2022
Total Project Value	$ 1,615,000
Technology Area	Plant Optimization Technologies

This project evaluating advanced nickel (Ni)-based alloys to support the manufacturing and use of components under advanced ultra-supercritical (AUSC) steam conditions, which range up to 760 degrees Celsius (°C; 1400 °F) and 35 megapascals (MPa; 5000 psig). In particular, this project focuses on evaluating materials from near-to-full-scale components, such as Haynes 282 large rotor forging, half-valve body casting, and steam turbine nozzle carrier casting, to provide (a) insights into potential manufacturability issues related to large-scale components made from Ni-based alloys and (b) engineering data and support for actual AUSC plant design. In addition, this project contains substantial efforts in weld characterization and long-term creep testing of Ni-based alloy weldment, which should provide useful data for filler metal selection and future ASME code qualification efforts for cast Haynes 282 weldment.



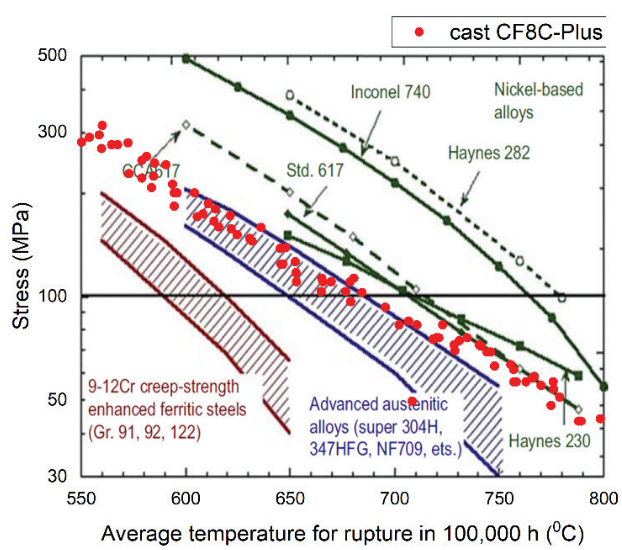
Cross-section view of creep rupture specimens of Inconel 740H cross-weld made with alloy 263 filler metal.

Low Cost High Performance Austenitic Stainless Steels for A-USC

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA133
Project Duration	10/01/2019 – 09/30/2022
Total Project Value	$ 1,590,000
Technology Area	Plant Optimization Technologies

This project evaluating the behavior of high-temperature materials to qualify low-cost alloys for steam turbine designs required for operation under advanced ultra-supercritical (AUSC) steam conditions (760 °C and 345 bar/1400 °F and 5000 psig steam), and in ensuring that any limitations of current materials are overcome. This project is focused on obtaining long-term creep properties of full- or near-full-sized components of extruded tubes and pipes or other parts fabricated from the CF8C-Plus alloy for component testing in an actual AUSC power plant environment (ComTest).

The key to enabling higher efficiencies/lower emissions is the availability of materials capable of operation in steam at the higher temperatures and pressures. In particular, the limiting temperature for current steam turbines is set by the strength of the material used for the turbine casings, which are constructed from large castings that have complex shapes to accommodate the turbine vanes and blades; typically, assembly involves welding together several castings. To meet these requirements, the alloy used must develop the required strength in the as-cast state (since the size of the castings and the large changes in section thickness restrict the ability to control post-casting heat treatments) and have good weldability. The alloys used for current steam turbine casings are 2-10%Cr ferritic steels, for which the maximum temperature capability is approximately 620 °C (1,148°F). For higher temperatures, austenitic steels typically are the next choice, but the thermal fatigue properties of most cast austenitic steels are unsuitable for this application. However, cast CF8C-Plus steel has outstanding fatigue and thermal fatigue resistance, so this steel might be useful for such applications.



Comparison of 100,000 h creep-rupture strength as a function of temperature between cast CF8C-Plus and other alloy classes.

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

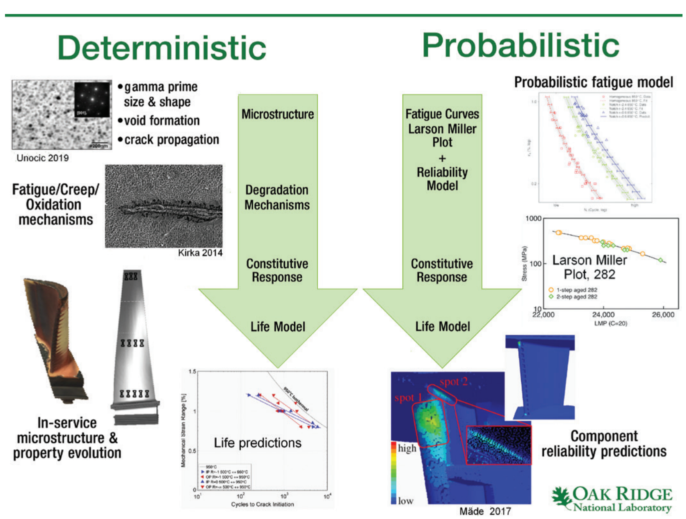
Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA137
Project Duration	10/01/2018 – 05/31/2022
Total Project Value	$ 900,000
Technology Area	Plant Optimization Technologies

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

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

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

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

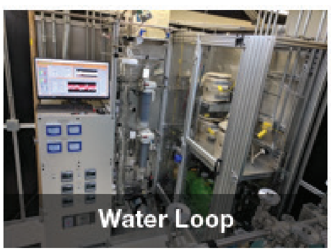


Steamside Oxidation Issues in Current Coal-Fired Boilers

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA150
Project Duration	08/01/2019 – 09/30/2022
Total Project Value	$ 900,000
Technology Area	Plant Optimization Technologies

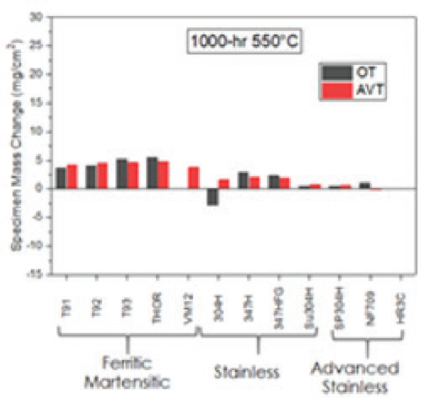
The primary goal of this project is to develop a steamside oxidation model that will incorporate important real-world parameters such as water chemistry, pressure, and scale adhesion for current coal-fired boiler systems and cover growth and exfoliation. The initial focus will be on evaluating the temperature-dependent effect of oxygen content and the role of amines on the oxide scale morphologies to enable a quantitative analysis of the adhesion and exfoliation behavior of both ferritic and austenitic steels. A better understanding of the underlying mechanisms will allow a realistic lifetime prediction of currently employed materials under a range of partial- and full-load duty cycles and suggest avenues for the deployment of surface modifications including coatings and shot peening.

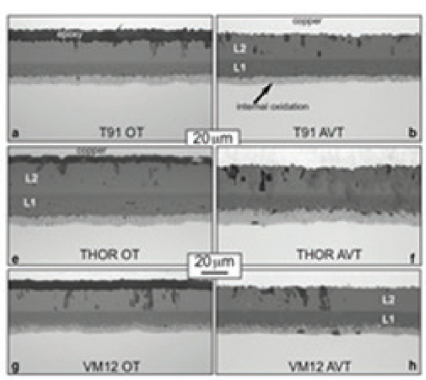
Testing



- 275 bar water, 50-h cycles, 550-650°C
- Feritic-martensitic and austentic steels
- **Controled water chemistry:** OT (100ppb O_2), AVT (<10 ppb O_2)
- **Additions:** 2 film forming products (amines)

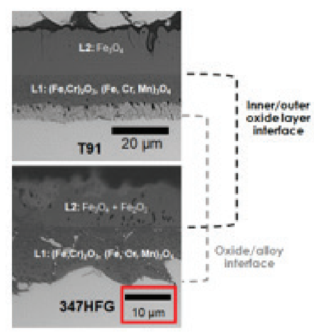
Oxidation Behavior

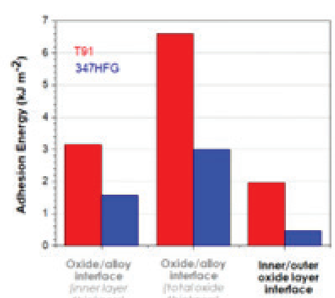




Water chemistry did not significantly influence specimen mass change

Microstructural Analyses





In-situ SEM tensile testing resulted in lowest adhesion energies for the inner/outer interference that coresponds well to observed failure interface

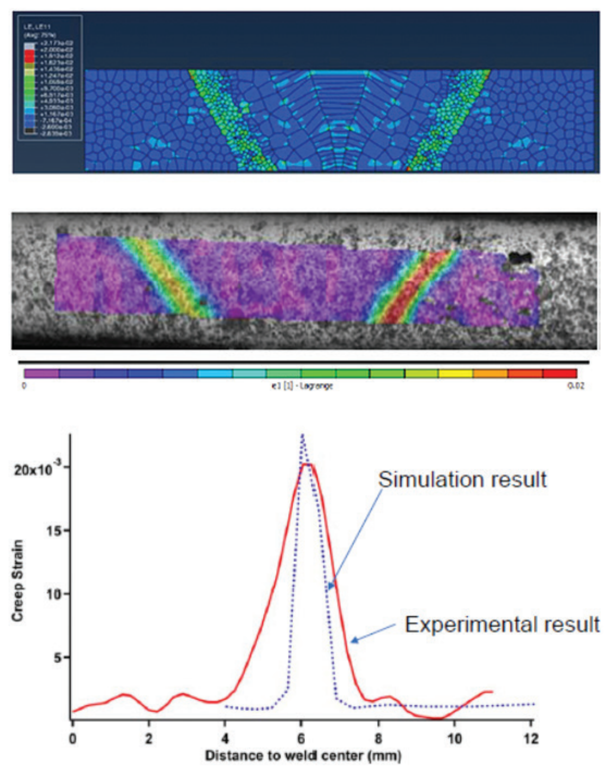
Weldability of Creep Resistant Alloys for Advanced Power Plants

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA118
Project Duration	10/01/2013 – 03/31/2022
Total Project Value	$ 1,800,000
Technology Area	Plant Optimization Technologies

NETL partnered with ORNL to develop practical engineering solutions to two key issues regarding the weldability of high-temperature creep-resistant alloys used in advanced fossil energy power plants: (1) the reduced creep strength of the weld region versus the base metal, and (2) welding of dissimilar metals.

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

The research will promote the design of advanced power plants capable of operating at higher temperatures and pressures, thus improving their efficiency and operational flexibility and reducing capital and operating costs.



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

COMPUTATIONAL MATERIALS DESIGN

eXtremeMAT: Extreme Environment Materials

Performer	**National Energy Technology Laboratory**
Award Number	FWP-1022433
Project Duration	10/01/2018 – 09/30/2022
Total Project Value	$ 2,496,921
Technology Area	Coal Utilization Science

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

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

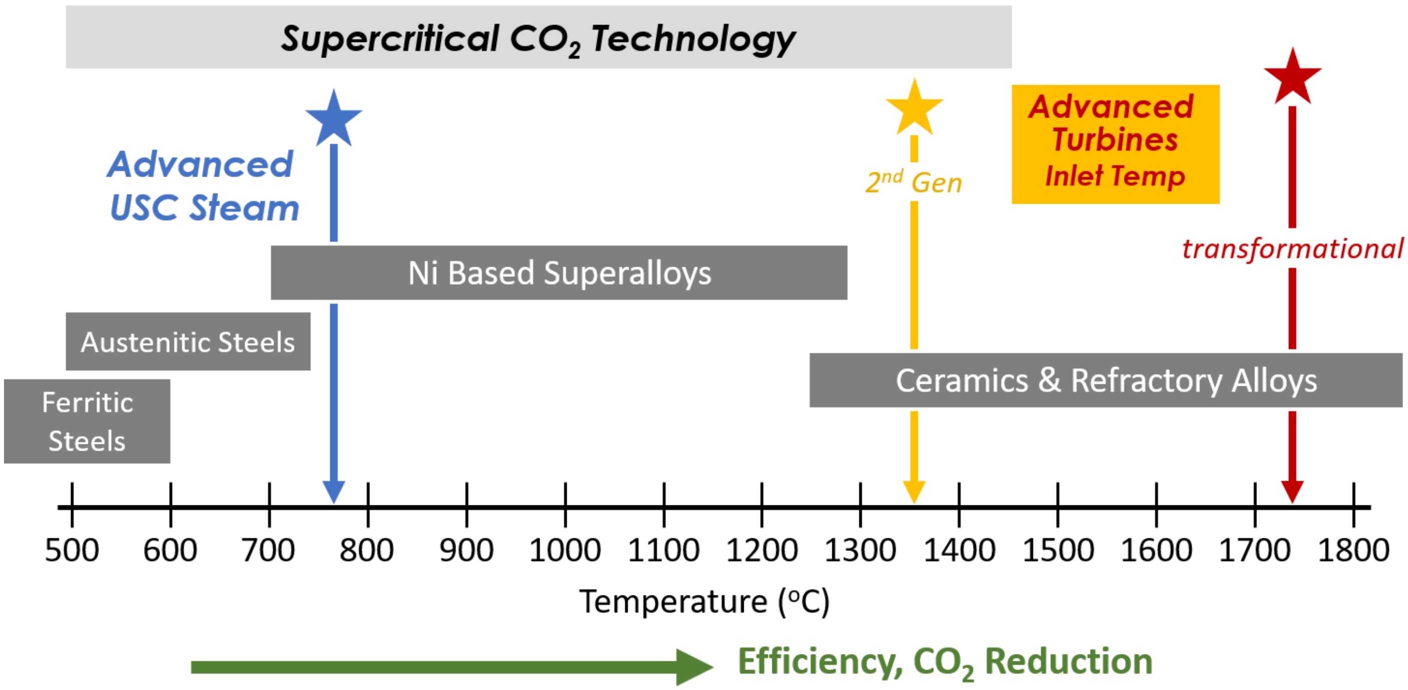
- Developing a suite of improved heat resistant alloys for fossil energy components in existing and future power plants
- Predicting long-term materials performance in existing and future fossil energy power cycles

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

Initially, the effort will target enabling sCO_2 technologies through the development of high yield strength, high-temperature austenitic stainless steel alloys. Although nickel (Ni) superalloys can meet the performance objectives of sCO_2 technologies, they are costly and may limit the broad application of these technologies. Improvements in the performance of austenitic stainless steels will enable a wider application of lower-cost alloys, thereby reducing the amount and cost of nickel required in the overall system. The challenge is to increase the yield and creep strength of austenitic steels to enable long-term operation at temperatures above 700 degrees Celsius, while maintaining low costs and manufacturability, using computational tools integrated with experimental characterization. While targeting austenitic alloys, the methodologies developed in this project will be applicable for developing new alloys or for improving the properties and performance of other lower-cost alloys such as 9–12 percent chromium steels and higher-performance alloys such as Ni-based or high-entropy alloys.

In the near term, the project team is working to identify promising candidates for new low-cost iron-based alloys that would perform well in an sCO_2 environment. In the long term, the team aims to develop and demonstrate a new approach to materials discovery and development for future energy applications. This approach would exploit multiscale (molecular-to-continuum) simulation methods to explore the performance of new materials over wide ranges of compositional space, identifying promising formulations for specific service conditions that can subsequently be tested at the bench scale. This requires overcoming major simulation challenges and confidently predicting both the properties of metallic alloys over wide ranges of compositional space and the performance life of these materials. If this can be demonstrated, the current laborious approach to materials discovery can be transformed and the path from materials discovery to commercial deployment can be dramatically accelerated.

Lastly, the ability to manufacture these new alloys at scale needs to be demonstrated and matured to a level that would encourage industrial adoption in the commercial application.



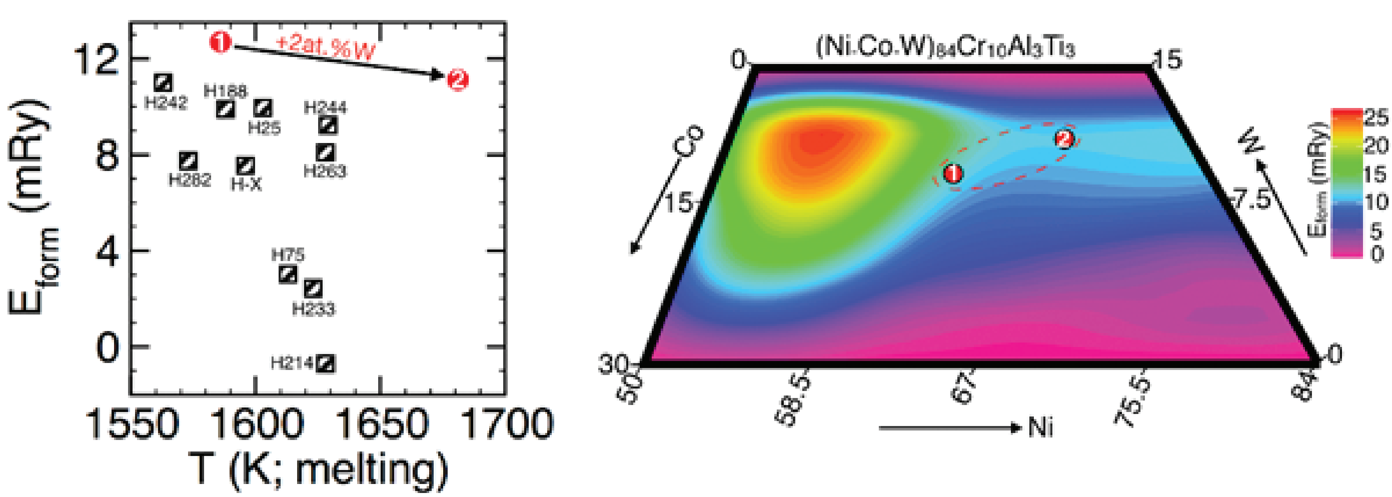
Extreme environment materials for advanced fossil energy power generation.

Predictive Design of Novel Ni-based Alloys

Performer	Ames National Laboratory
Award Number	FWP-AL-19-510-097
Project Duration	04/08/2019 – 06/30/2022
Total Project Value	$ 750,000
Technology Area	Plant Optimization Technologies

Ames National Laboratory's (Ames) goal is to increase operating temperatures of the Ni-based superalloys through controlled alloying additions. Additions will be chosen using a three-pronged approach: (i) alloying additions aimed at preventing the formation of topologically close-packed (TCP) phases, (ii) improving the liquidus temperature of the gamma phase, and (iii) preventing microstructural coarsening by improving the microstructural stability of the gamma prime phase. Beyond the effect of alloying additions and processing on the melting temperatures, Ames will investigate the effect of alloying additions on the alloy's high-temperature oxidation resistance. Differing from a number of traditional approaches to high-temperature oxidation, recession rates rather than parabolic kinetics will be employed to ascertain the oxidation resistance. Once precipitation and coarsening kinetics are established for given chemistries and temperature, a regression-decision approach will be developed for creating an optimization "surface" of alloy design parameters (chemistry, processing parameters, and desired melting/liquidus temperatures and oxidation resistance) enabling optimization of the Ni-based alloys.

Thus, Ames will develop a novel alloy design and optimization strategy for Ni-based alloy systems that establishes the interrelation between alloying additions, processing conditions, and performance metrics. The approach is based on destabilization of deleterious phases through alloying additions, while controlling the microstructure and near-surface chemistries to design an oxidation-resistant high-temperature alloy.



Left chart shows how E_{form} varies with experimentally determined T_m for common Haynes alloys. Right graphic shows (on a reduced pseudo-quaternary plot) how E_{form} varies with content of the refractory element; W, with Ni and Co.

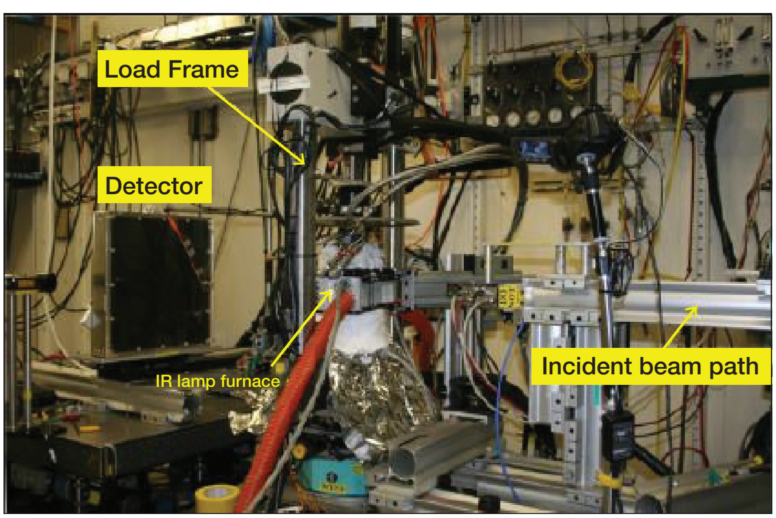
Damage Accumulations Predictions for Boiler Components Via Macrostructurally Informed Material Models

Performer	**General Electric (GE) Company**
Award Number	FE0031823
Project Duration	10/01/2019 – 09/30/2022
Total Project Value	$ 907,084
Collaborator	Energy Industries of Ohio
Technology Area	Plant Optimization Technologies

The goal of this project is to develop accurate models of the physical and mechanical behavior and degradation of nickel-based superalloys during cyclic operations in fossil energy power plants where thermo-mechanical fatigue and creep damage are occurring at the same time. The project will build on knowledge and models developed in previous DOE-funded projects to expand current microstructure-based models and predict hold time cyclic loading for nickel-based superalloy Haynes 282 at temperatures between 1100 and 1400 degrees Fahrenheit. Enhanced material model capabilities will be demonstrated by analyzing a superheater header component, comparing total strain evolution in time in the highest-strained regions for various wall thicknesses.

The project focus is on an alloy (Haynes 282) that is increasingly used in boiler and piping components of fossil power plants. Researchers will provide physically informed models, capturing the microstructural changes taking place in components under cyclic loading and exposure to high stress and temperature for operating life up to 300,000 hours.

Validated software tools will be developed that can be used to increase accuracy in predicting the life of high-temperature nickel components in the long term and subject to significant cycling operation as well as to improve the design of new high-temperature components for new power plants or for use in existing power plants.



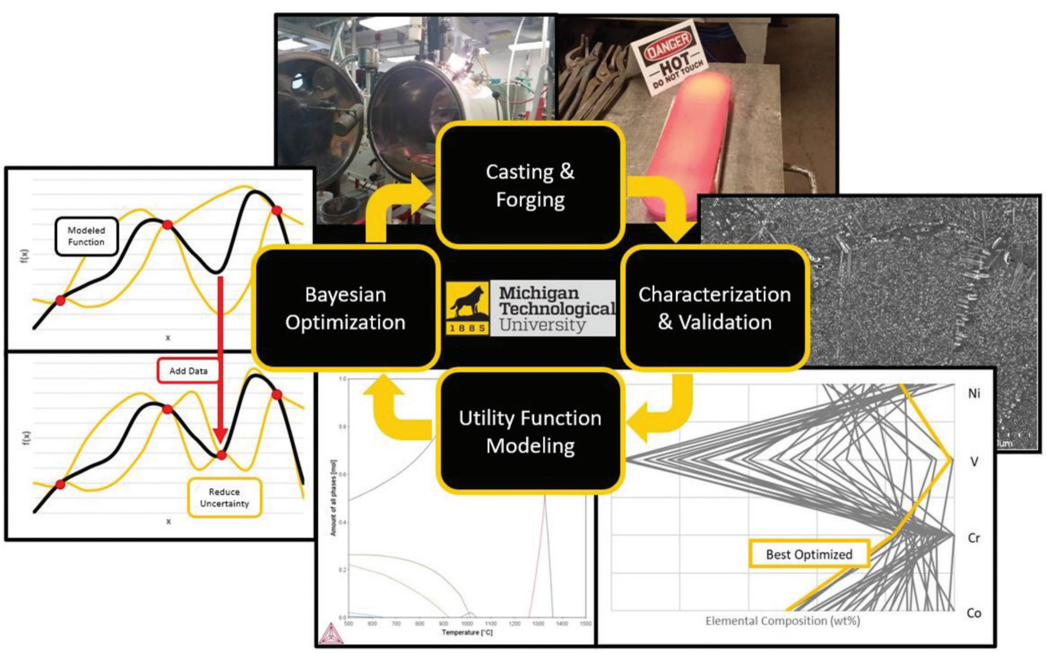
Cyclic loading test setup.

Hybrid Structured Nickel Superalloys to Address Price Volatility and Weld/Weld Repair Based Supply Chain Issues

Performer	**Michigan Technological University**
Award Number	FE0032071
Project Duration	09/03/2021 – 09/02/2024
Total Project Value	$ 400,000
Technology Area	University Training and Research

Two key factors affecting the fossil power high-temperature material supply chain are the volatility of nickel-based alloy prices and the challenges in welding precipitation-strengthened alloys. This project seeks to use integrated computational materials engineering (ICME) design strategies to solve these challenges by designing, casting, forging, welding, and validating the properties of hybrid eta-gamma prime-strengthened nickel superalloys optimized for cost and weldability. Specifically, significant reduction in cobalt to less than 5 wt.% versus 10–20% in candidate alloys for advanced energy systems is sought. Performance in high-temperature strength and creep will be maintained within 10% compared against existing candidate alloys designed for extreme environments. Weldability criteria will be evaluated through use of various susceptibility indices (solidification cracking, liquation, stress relief cracking) with the goal of broadening the welding and post-weld heat treat processing windows to be more forgiving.

Benefits are focused on providing alternatives to existing alloys with significant weldability issues which will enhance fabrication of new components, on-site assembly, and in-service repairs. Additional impacts include training graduate students in "hybrid" real-world/theoretical design methodologies to better prepare for advanced materials development.



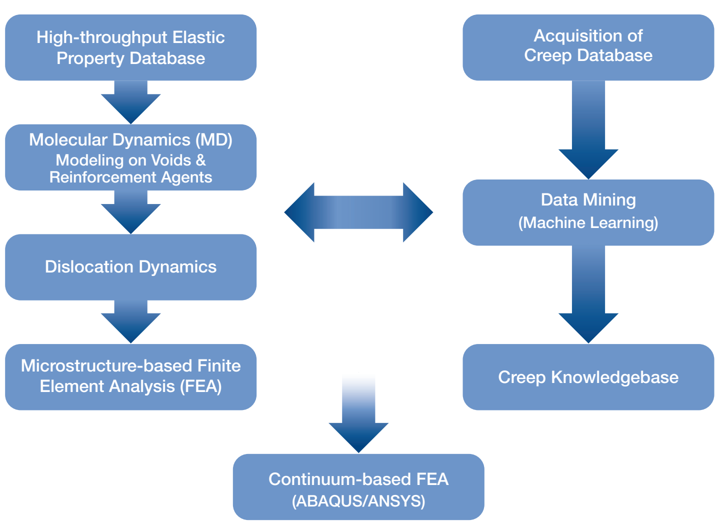
Michigan Technological University's Experimental Process.

Multi-modal Approach to Modeling Creep Deformation In Ni-Base Superalloys

Performer	**Missouri State University**
Award Number	FE0031554
Project Duration	12/15/2017 – 12/14/2021
Total Project Value	$ 918,370
Collaborators	Missouri University of Science and Technology; University of Missouri–Kansas City
Technology Area	Plant Optimization Technologies

NETL partnered with Missouri State University to develop a new multi-modal approach to modeling of creep deformation in nickel-base superalloys. The approach is based on a two-pronged strategy combining a bottom-up, multi-scale, physically based modeling approach and a data-mining-driven top-down approach, backed by experimental database and correlation connectivity with strength augmented by data mining/machine learning protocols. The overarching goal is to integrate these two strategies to create quantitatively better predictive creep models that are not only sensitive to the microstructural evolution during various stages of creep, but also based on physically sound creep modeling that judiciously encompasses the strength of each modeling scale and provides a more comprehensive creep deformation analysis via finite element analysis.

The main advantage of the project's approach is to establish a new framework within which the adaptation of data mining tools for predicting the creep property of nickel-base alloys can be accelerated using a rigorous step-by-step atomistic-mesoscale continuum-based simulation. This approach will reduce the level of uncertainty of experimental creep data and facilitate a better linkage between the experimentally acquired creep data and the creep models that are established through the hierarchical multi-scale modeling. Ultimately, it will provide better diagnostics on the slow progression of creep deformation and will help to improve the quantitative predictive capability for the onset of creep failure during the tertiary creep stage. The approach can also be applied to a wider range of material candidates for fossil energy power plants.



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

Advanced Alloy Development

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022406
Project Duration	04/01/2018 – 03/31/2023
Total Project Value	$ 13,359,337
Technology Area	Plant Optimization Technologies

NETL's Research and Innovation Center's Advanced Alloy Development Field Work Proposal (FWP) is focused on developing high-performance materials to improve efficiencies in the existing fleet and enable advanced fossil energy systems. NETL uses an integrated materials engineering approach that incorporates computational alloy design with best-practice manufacturing (modified as needed to achieve microstructure and performance objectives) with focused performance evaluation and characterization. Research is conducted to develop and validate computational algorithms for designing advanced alloys and for predicting alloy performance over multiple length scales and multiple time scales relevant to advanced fossil energy power systems.

The Advanced Alloy Development FWP has five distinct research themes:

Systems Engineering & Analysis (SE&A)—Provide techno-economic and market studies on fossil fuel power generation plants operating at the elevated conditions [e.g., advanced ultrasupercritical (AUSC) Rankine cycles] enabled by advanced alloys, identifying applications, and quantifying the cost and performance improvements relative to the commercial state of the art.

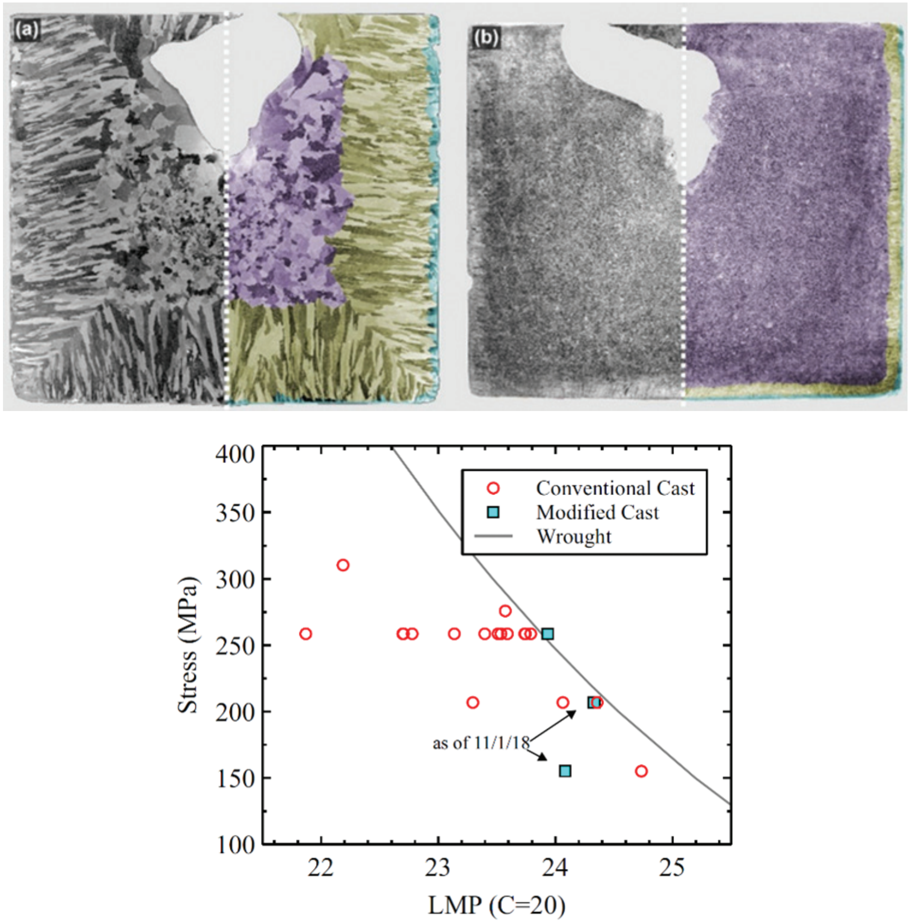
Computational Design and Simulation—Use computational materials modes, multi-scale characterization simulations of microstructural features, and cutting-edge data analytics to guide and accelerate alloy design and manufacturing development.

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

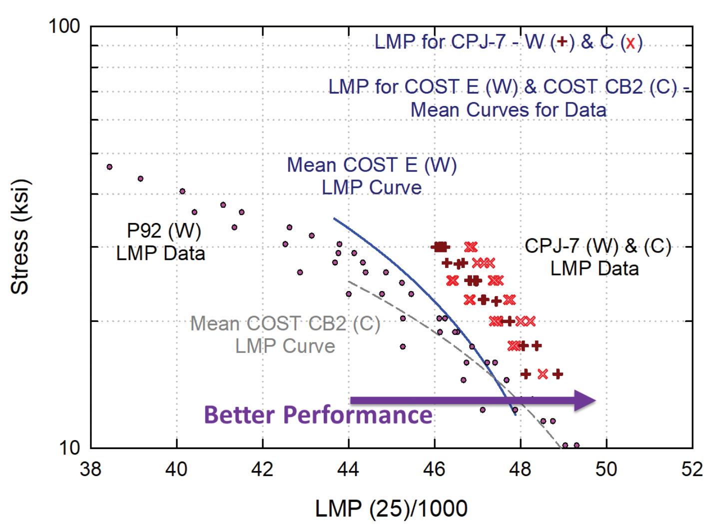
Materials for sCO_2 Power Cycles: Alloy Performance—Determine whether available AUSC power plant materials are suitable for fossil fuel supercritical carbon dioxide (sCO_2) service in terms of temperature and stress, and if they are, assess the potential physical and mechanical consequences of their use.

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

The structural materials and manufacturing processes researched in this FWP are needed to lower the cost and improve the performance of fossil-based power-generation. Additionally, the development and utilization of computational simulation and broad-based data analytic tools can further reduce the time and cost of developing advanced energy systems.



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



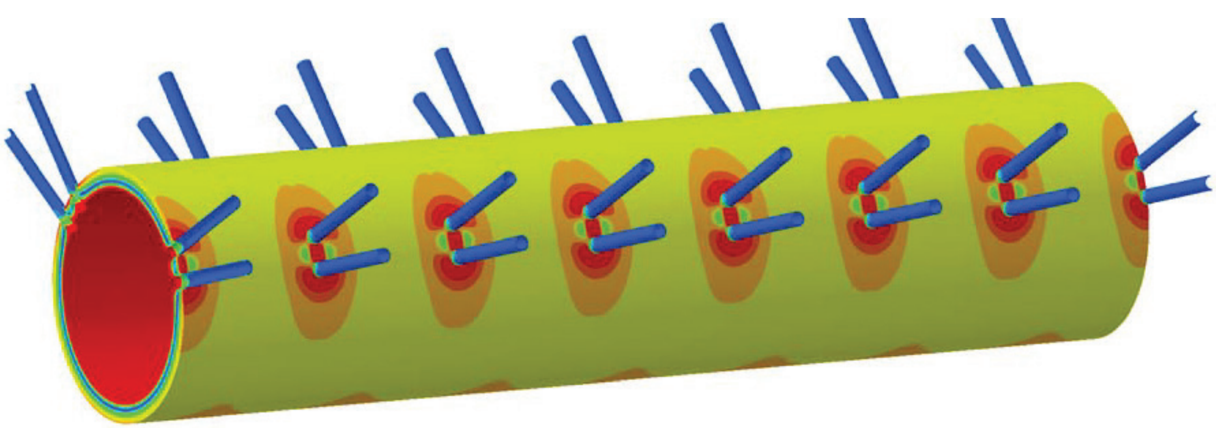
Creep behavior: NETL's CPJ-7 compared to other advanced Fe-9Cr streels, COST E, Cost CB3 and P92. W=Wrought, C=Cast.

Alloy for Enhancement of Operational Flexibilty of Power Plants

Performer	**North Carolina Agricultural and Technical State University**
Award Number	FE0031747
Project Duration	08/15/2019 – 08/14/2022
Total Project Value	$ 400,000
Collaborator	University of North Carolina Charlotte
Technology Area	University Training and Research

North Carolina Agricultural and Technical State University will employ advanced computational techniques to address the challenge of higher material deterioration facing existing coal-fired power plants due to a shift in their operational mode from baseline steady state to cycling. The cycling operation of coal-fired power plants promotes thermo-mechanical fatigue damage in boiler headers. As a result, materials deteriorate at a higher rate and ligament cracking occurs in headers in a shorter time. The main objective of this project is to employ computational fluid dynamics and finite element analysis to conduct a comprehensive and advanced study of the applicability of Inconel (IN) 740H superalloy in steam headers to improve the operating flexibility of power plants. The project team will use the results of the analysis to optimize the geometry of headers to minimize the quantity of material used.

A cost-benefit analysis of headers designed with IN740H (employing both traditional and optimized shapes) in comparison with creep-strength-enhanced ferritic (CSEF) steels such as Grade 91 will be conducted. This analysis will consider the higher cost of IN740H with respect to CSEF steels and the lower maintenance cost of IN740H during operation of the power plant.



Stress contour plot of a steam header.

High-Speed and High-Quality Field Welding Repair Based on Advanced Non-Destructive Evaluation and Numerical Modeling

Performer	Ohio State University
Award Number	FE0032067
Project Duration	09/24/2021 – 09/23/2024
Total Project Value	$ 400,000
Technology Area	University Training and Research

The goal of the project is to establish the experimental and computational foundations that are crucial to implement high-speed and high-quality field welding repair based on advanced non-destructive evaluation (NDE) and numerical modeling. The scope of work of the project is focused on developing two enabling techniques for repair of CSEF Grade 91 and 92 steel components: (1) microstructure detection using ultrasonic NDE, and (2) hardness prediction using a computational model for multi-pass, multi-layer welding.

Weld coupons will be fabricated using a high-deposition-rate process based on hot wire gas tungsten arc welding (GTAW). These weld coupons will be characterized for microstructure and hardness, which provides the baseline data for Gleeble® physical simulation to produce a bulk weld microstructure. Through the control of peak temperature and time, individual microstructures (especially martensite) with different levels of tempering will be produced. This simulated microstructure is needed since the actual weld comprises a highly inhomogeneous microstructure that is difficult for analysis by raw ultrasonics. Samples containing different microstructures will be scanned using ultrasonic testing and advanced data processing algorithms such as machine learning will be used to find ultrasound parameters that are unique to the susceptible microstructures. The physics-based models will consider the heat transfer and molten pool fluid flow in a multi-pass, multi-layer dissimilar metal welding repair. The Gleeble testing results will also be used to develop a tempering kinetic model to predict the as-welded hardness distribution as well as that after post-weld heat treatment (PWHT).

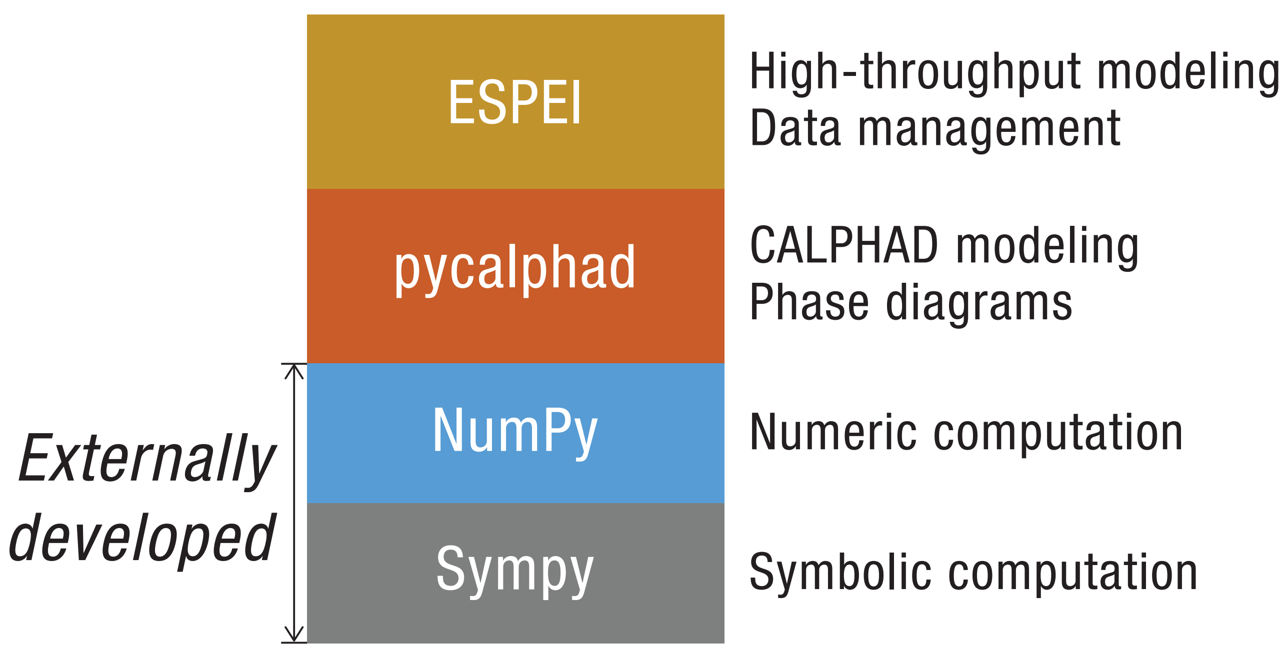
High-quality field welding repairs on CSEF steel components are critical to the reliable and efficient operation of the current fleet of power plants in the United States. Development of a reliable field-usable NDE technique will ensure that the required microstructure is achieved after onsite welding. Additionally, establishing knowledge of weld reparability for newer CSEF steels such as Grade 92 based on advanced numerical models of welding processes will facilitate their adoption. The tools and knowledge to be generated in the project will establish experimental and computational foundations to achieve the overall goal of detecting and controlling microstructure and properties for welding repair onto CSEF steel components.

High Throughput Computational Framework of Materials Properties for Extreme Environments

Performer	**Pennsylvania State University**
Award Number	FE0031553
Project Duration	12/15/2017 – 12/14/2021
Total Project Value	$ 937,836
Technology Area	Plant Optimization Technologies

NETL partnered with Pennsylvania State University to establish a framework capable of efficiently predicting the properties of structural materials for service in harsh environments over a wide range of temperatures and long periods of time. The approach is to develop and integrate high-throughput first-principles calculations based on density functional theory in combination with machine learning methods, perform high-throughput calculation of phase diagrams (CALPHAD) modeling, and carry out finite-element method simulations. In regard to high-temperature service in fossil power systems, nickel-based superalloys Inconel 740 and Haynes 282 will be investigated.

The framework has the potential to enable high-throughput computation of tensile properties of multi-component alloys at elevated temperatures, resulting in significant reduction in computational time needed by the state-of-the-art methods. Once successfully completed, the project will deliver an open-source framework for high-throughput computational design of multi-component materials under extreme environments. This framework will enable more rapid design of materials and offer the capability for further development of additional tools due to its open-source nature.



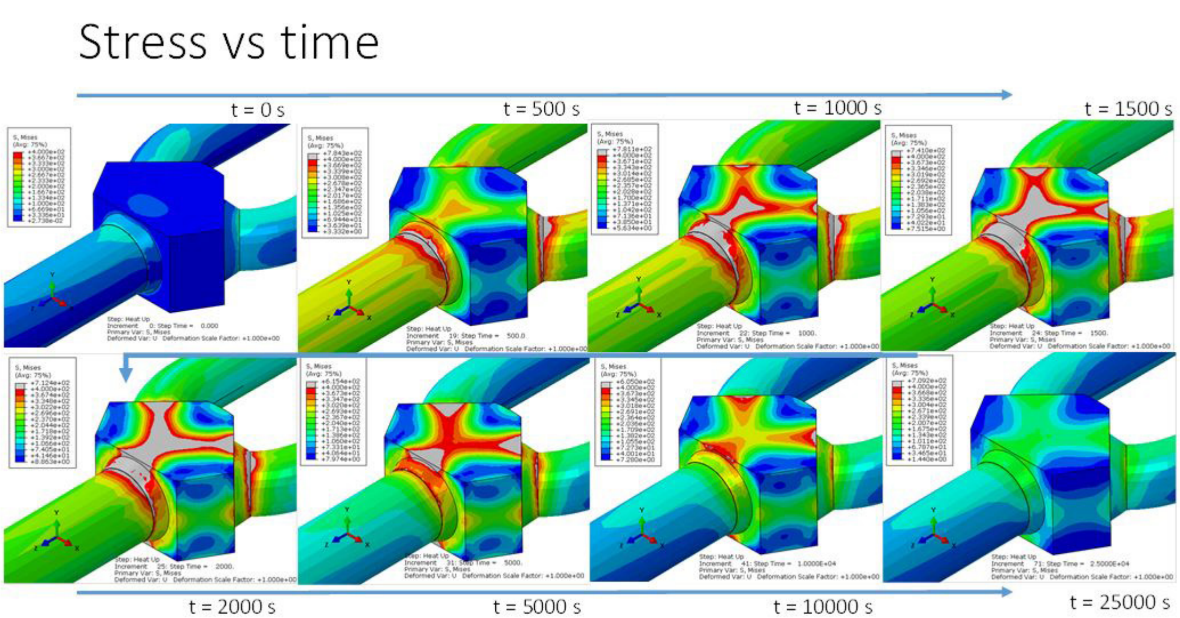
ESPEI-2.0 software stack.

Life Modelling of Critical Steam Cycle Components in Coal- Fueled Power Plants

Performer	Southern Research Institute
Award Number	FE0031811
Project Duration	10/01/2019 – 09/30/2022
Total Project Value	$ 862,345
Technology Area	Coal Utilization Science

Southern Research Institute will calibrate an existing damage accumulation and component life model to a high-pressure turbine disk/rotor alloy (used in a steam-cycle turbine of a coal-fueled plant) and a steam-cycle Y-block alloy. The component life model that will be calibrated accounts for coupled thermomechanical damage accumulation, material microstructural evolution, and material or component erosion or corrosion damage to determine component life predictions. The damage accumulation model, complete with lifetime prediction capabilities, will be implemented in Microsoft Excel or MATLAB format, and will only require particular input data such as inelastic strain, hydrostatic stress, temperature-time waveforms, initial microstructure, etc., from a component-specific finite element analysis, to predict component lifetime. The work will be performed in conjunction with Southern Company, an industry partner and owner of a coal-fueled power plant. The project will include four primary tasks: (1) project management and planning, (2) materials characterization, (3) damage model calibration, and (4) component life model calibration and verification. The primary goal is to provide calibrated life estimation models for a DR22 steel Y-block and a Jethete stainless steel turbine blade.

The tool developed will enable lifetime prediction as a function of historical plant steam-cycle operational data as well as any potential proposed future operational cycling. Consequently, existing coal-fueled power plants will be able to operate safely for longer periods of time and at higher efficiencies, thereby reducing the economic and environmental impact of the existing coal power plant fleet.

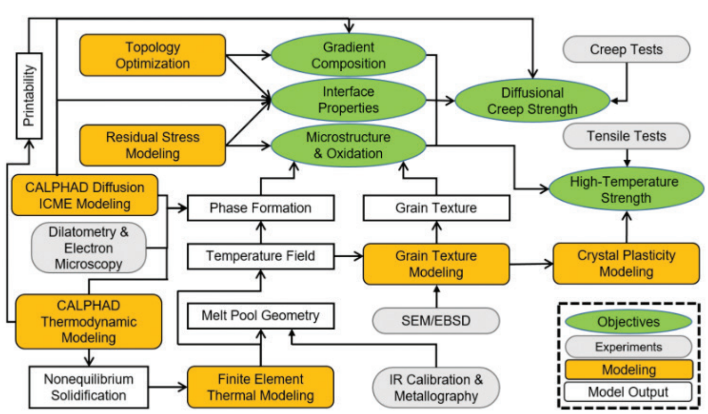


Integrated Computational Materials and Mechanical Modeling for Additive Manufacturing of Alloys with Graded Structure used in Fossil Fuel Power Plants

Performer	**University of Pittsburgh**
Award Number	FE0031637
Project Duration	11/01/2018 – 10/31/2021
Total Project Value	$ 937,500
Collaborator	United Technologies Research Center
Technology Area	Coal Utilization Science

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

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



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

HYDROGEN PRODUCTION

Electromagnetic Energy-Assisted Thermal Conversion of Fossil-Based Hydrocarbons to Low-Cost Hydrogen

Performer	**University of North Dakota**
Award Number	FE0032061
Project Duration	08/01/2021 – 07/31/2023
Total Project Value	$ 398,969
Technology Area	University Training and Research

Hydrogen can be produced from the decomposition of hydrocarbons such as methane, without the production of carbon oxides. This represents a highly favorable route for hydrogen production compared to industrial production methods based predominantly on steam-methane reforming (SMR). Breaking hydrogen-oxygen bonds in water requires about seven times the energy compared to breaking carbon-hydrogen bonds in methane. SMR and methane decomposition processes both require indirect heating to provide the overall endothermic heat of reaction for hydrogen formation, but the heat of reaction for the SMR is more than double that for methane decomposition. In contrast to the SMR process, the methane decomposition process offers a promising path for economical and environmentally sound production of hydrogen without production of carbon dioxide.

The goal of this project is to make targeted improvements to the conventional thermo-catalytic hydrocarbon conversion process using an electromagnetic energy assisted mechanism; resulting in the reduction of downtime associated with catalyst reactivation or replacement due to poisoning. State-of-the-art solid catalysts exhibit short process lifetimes that are not suitable for commercial application. This project uses both experimental and computational tools to understand the fundamental interactions between fossil fuels and their interactions with an electromagnetic energy source. This technology can utilize natural gas or volatiles obtained from coal decomposition to provide carbon dioxide-free hydrogen. The first objective of this project is to identify catalyst supports that enhance the electromagnetic energy-assisted mechanism to ensure in-situ catalyst reactivation to near-initial fresh conditions. The performance of these prepared catalysts will be tested in laboratory units and the results will be used to validate computational fluid dynamics (CFD) and chemical kinetics models. Finally, CFD will be used to investigate the electromagnetic energy-assisted conversion mechanism as a function of catalyst structure and operating conditions for hydrogen production.

This study will provide future researchers with a cost-effective tool to explore a multitude of yet-to-be-conceived electromagnetic systems to ensure long-term catalytic activity. The technology has the potential to extend the longevity of catalyst materials, thereby reducing overall catalyst replenishment costs. With these improvements to the conventional thermo-catalytic hydrocarbon conversion process, it is hoped to enable a wider adoption of hydrogen-related technologies from fossil resources. This project will also support two graduate students focused on fossil energy research.

ABBREVIATIONS

°C .... degrees Celsius
°F .... degrees Fahrenheit
AM .... additive manufacturing
AM-GCTJ .... additively manufactured graded composite transition joint
ASME .... American Society of Mechanical Engineers
ALD .... atomic layer deposition
AUSC .... advanced ultrasupercritical
CALPHAD ... calculation of phase diagrams (methodology)
CFD .... computational fluid dynamics
Co .... cobalt
CO_2 .... carbon dioxide
Cr .... chromium
CSEF .... creep strength enhanced ferritic
Cu .... copper
DFT .... density functional theory
DFTB .... density functional tight binding
DMW .... dissimilar metal weldments
DOE .... Department of Energy
EEM .... extreme environment material
$Er2O_3$ .... erbium
FECM .... DOE Office of Office of Fossil Energy and Carbon Management
Fe .... iron
FWP .... Field Work Proposal
GB .... grain boundary
GPU .... graphics processing unit
H282 .... Haynes 282
H_2O .... water
HBCU .... Historically Black Colleges and Universities
HP .... high-pressure
HPM .... High Performance Materials
ICME .... integrated computational materials engineering
ICWE .... integrated computational welding engineering
IN .... Inconel
IN740H .... Inconel 740H
INL .... Idaho National Laboratory
IPD .... ion plasma disposition
LP .... laser processing
ML .... machine learning
Mn .... manganese
MPa .... megapascals
NETL .... National Energy Technology Laboratory
Ni .... nickel
NNS .... near net shape
O_2 .... oxygen (molecular)
ODS .... oxide dispersion strengthened
OMI .... Other Minority-Serving Institutions
ORNL .... Oak Ridge National Laboratory
Pitt .... University of Pittsburgh
PM .... powder metallurgy
PNNL .... Pacific Northwest National Laboratory
psi .... pounds per square inch
psig .... pounds per square inch gauge
PWHT .... post-weld heat treatment
R&D .... research and development
sCO_2 .... supercritical carbon dioxide
SMR .... steam-methane reforming
SwRI .... Southwest Research Institute
TiO .... titanium oxide
TTU .... Texas Technological University

ABBREVIATIONS

UCFER .... University Coalition for Fossil Energy Research

UCR .... University Coal Research

UTRC .... United Technologies Research Center

WAAM .... wire-arc additive manufacturing

γ' .... gamma prime

η .... eta

NOTES

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WEBSITES:

https://netl.doe.gov/carbon-management/high-performance-materials

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

https://netl.doe.gov/carbon-management/crosscutting

https://www.energy.gov/fecm/science-innovation/office-clean-coal-and-carbon-management/crosscutting-research/plant

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