

# HIGH PERFORMANCE MATERIALS PROJECT PORTFOLIO 2021



U.S. DEPARTMENT OF  
**ENERGY**



NATIONAL  
ENERGY  
TECHNOLOGY  
LABORATORY

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## INTRODUCTION

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 six primary research areas: High Performance Materials; Sensors, Controls, and Novel Concepts; Simulation-Based Engineering; Water Management; 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<sub>2</sub>) 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 improves fossil energy power generation with sensors, distributed intelligent control systems, and increased security. Advanced sensors and controls provide pivotal insights into optimization of plant performance and increasing plant reliability and availability. NETL tests and matures novel sensor and control systems that are operable in power plants and capable of real-time measurements and that can improve overall plant efficiencies and allow for more effective ramp rates. Given the crosscutting nature of sensors and controls, these technologies will benefit power plants across the spectrum of fossil generation and other harsh-environment applications.

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, Robotics-based Inspection, Advanced Controls and Cyber Physical Systems (Distributed Intelligent Controls), and Cybersecurity/Blockchain.

**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.

**Water Management:** Water Management addresses competing water needs and challenges through a series of dynamic and complex models and analysis that are essential in informing and deciding between priority technology R&D initiatives. The program encompasses the need to minimize any potential impacts of power plant operations on water quality and availability. Analyzing and exploring plant efficiency opportunities can reduce the amount of water required for fossil energy operations.

New water treatment technologies that economically derive clean water from alternative sources will allow greater recycling of water within energy extraction and conversion as well as carbon storage processes. This helps reduce the amount of total water demand within fossil energy generation.

The program leads a critical national effort directed at removing barriers to sustainable, efficient water and energy use; developing technology solutions; and enhancing the understanding of the intimate relationship between energy and water resources. Water Management R&D focuses its research in three chief areas: increasing water efficiency and reuse, treatment of alternative sources of water, and energy-water analysis. These research areas encompass the need to minimize potential impacts on water quality and availability.

**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 coal science. 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 three research areas within HPM:

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

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 32 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

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

<b>Performer</b>	ASME Standards Technology, LLC
<b>Award Number</b>	FE0031933
<b>Project Duration</b>	09/26/2020 – 03/31/2022
<b>Total Project Value</b>	\$ 382,451
<b>Technology Area</b>	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<sub>2</sub>. 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<sub>2</sub>)
- 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.



Reporting Annual/Long-Term Heat Rate & lbm CO<sub>2</sub>/MWh.

## Low-Cost HIP Fabrication of Advanced Power Cycle Components and PM/Wrought IN740H Weld Development

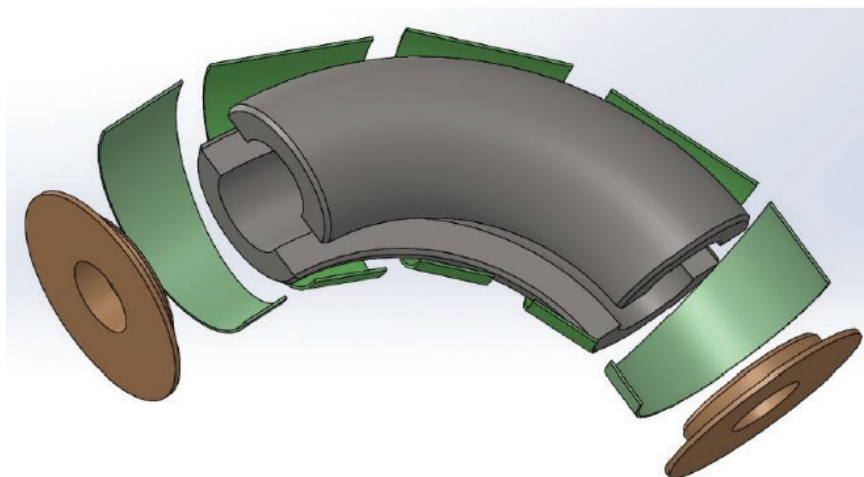
<b>Performer</b>	General Electric (GE) Company
<b>Award Number</b>	FE0031818
<b>Project Duration</b>	10/01/2019 – 06/30/2021
<b>Total Project Value</b>	\$ 1,299,505
<b>Collaborators</b>	Electric Power Research Institute, Inc.; Special Metals; Wyman-Gordon
<b>Technology Area</b>	Plant Optimization Technologies

The goal of this project is to demonstrate the feasibility of structures and components for advanced fossil energy power cycles by fusion welding powder metallurgy (PM) based near net-shape (NNS) hot isostatic pressed (HIP) nickel superalloy Inconel 740H (IN740H) components to cast or wrought IN740H components. Preliminary calculations indicate that structures fabricated by this method might reduce manufacturing costs by up to 50 percent, which would be approximately equivalent to a reduction in capital costs of \$13/kW and \$115/kW for fossil energy advanced ultra-supercritical (AUSC) steam Rankine cycle or supercritical carbon dioxide (sCO<sub>2</sub>) power plants, respectively.

The scope of work will first be to determine the powder characteristics of IN740H, which to date has not been produced in powder form. Compressive yield strength as a function of density and strain rate at multiple temperatures

will be measured. Physical properties and the prior particle boundary (PPB) particle network as a function of HIP cycle process parameters will also be evaluated. These results will then be used in a HIP process simulation model and other HIP process design tools in an integrated computational materials engineering framework to design the HIP capsule tooling to fabricate a prototype 150 lb Schedule 160 pipe elbow. After the near net-shape pressing process, the elbow will be machined to final dimensions and surface finish specifications. Welding process parameters will also be developed for joining IN740H PM based components to IN740H wrought components.

The technical data obtained from the fabrication of the IN740H NNS HIP 150 lb Schedule 160 pipe elbow will be used to develop a more accurate manufacturing cost model, which will increase the accuracy of cost estimates of NNS HIP components for AUSC power plant components.



Virtual assembling of the HIP tooling for the IN740H pipe elbow.



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

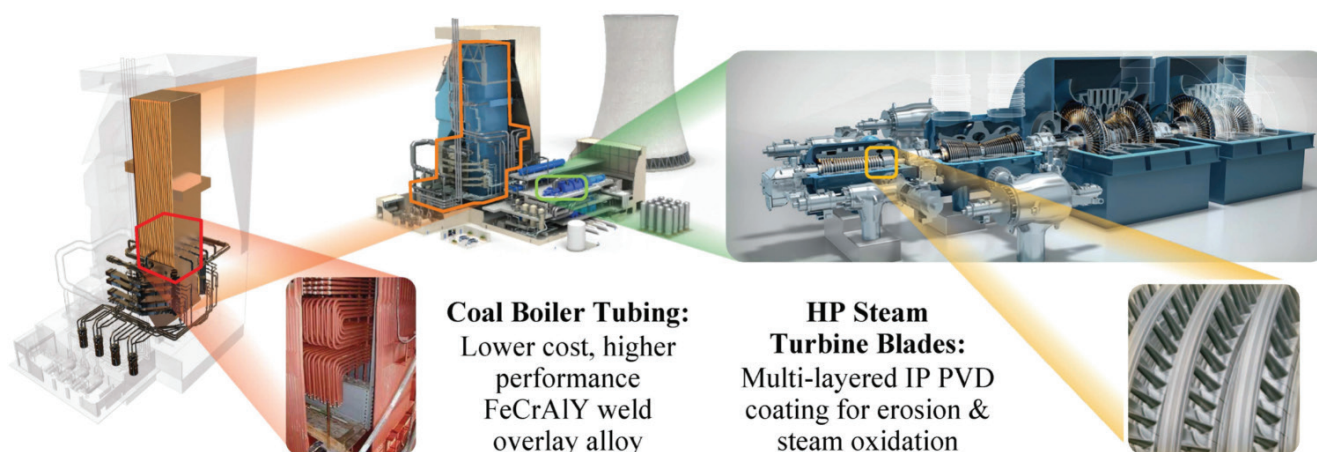
<b>Performer</b>	General Electric (GE) Company
<b>Award Number</b>	FE0031911
<b>Project Duration</b>	09/01/2020 – 08/31/2023
<b>Total Project Value</b>	\$ 5,549,995
<b>Technology Area</b>	Plant Optimization Technologies

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 Ni content in weld overlay to mitigate cost.
- Provide adequate oxidation resistance for HP turbine inlet steam at  $>620^{\circ}\text{C}$  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.



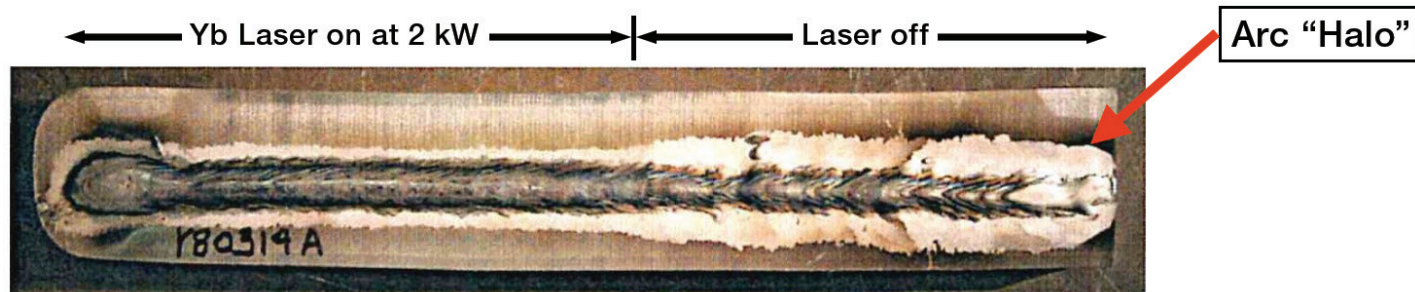
## Multi-pass Hybrid Laser Arc Welding of Alloy 740H

<b>Performer</b>	Idaho National Laboratory (INL)
<b>Award Number</b>	FWP-B100-19010
<b>Project Duration</b>	10/01/2019 – 09/30/2022
<b>Total Project Value</b>	\$ 1,294,000
<b>Technology Area</b>	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.

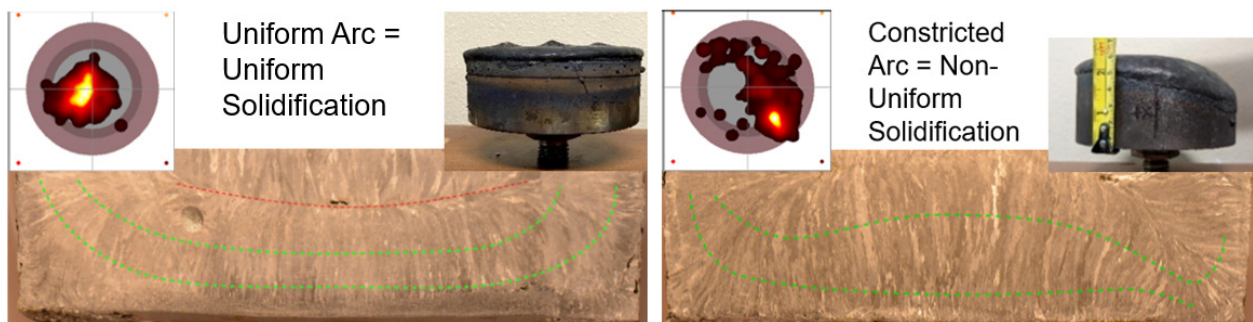
## Reducing the Cost of Ingots Utilized in Large Steam Cycle Components by Heat Flux Manipulation during VAR Processing to Control Solidification

<b>Performer</b>	Ampere Scientific
<b>Award Number</b>	SC0020980
<b>Project Duration</b>	06/29/2020 – 06/28/2021
<b>Total Project Value</b>	\$ 256,273
<b>Technology Area</b>	Plant Optimization Technologies

The objective of this project is to develop an approach to manufacture gamma prime strengthened superalloy (e.g., Inconel 740H) ingots in such a manner as to reduce the instances of defects while growing the diameter of the ingot to meet the needs of advanced power generation cycles. By combining an advanced measurement system with the application of transverse magnetic forces during vacuum arc remelting (VAR) processing, the solidification profile in ingots can be tailored. Specifically, Ampere Scientific will validate the applicability of a coupled measurement and control system by a) investigating system dynamics during experimental VAR operations to validate their measurement technology under superalloy processing conditions (short arc gaps influenced by drip short dynamics), b) verifying that the low current profiles during the melting of these alloys can be influenced by the application of transverse magnetic fields, and c) developing an arc gap measurement technique to overcome the limitations in the current drip-short controlled measurements. The culmination of these

three investigations provides the basis for simultaneously growing larger superalloy ingots while increasing yield, thus decreasing processing costs. To this end, the following three tasks will be accomplished during the Phase I work: a) modify an existing VAR system to sustain the necessary melting conditions required for experimental validation of the approach, b) validate arc gap tracking and arc gap length measurement, and c) analyze data to establish the relationship between arc conditions and defect generation.

The technology has commercial application to VAR and electro-slag remelting facilities in the United States and throughout the world. In particular, the melting of almost all specialty metals and many highly alloyed steels are manufactured in these furnaces, which have not significantly changed in more than four decades. The beneficiaries of this effort are the ingot producers and their customers, and the consumer through the availability of electricity from advanced generation systems.



Ingots sections identifying the microstructural differences between uncontrolled (left) and controlled arc dynamics. In the uncontrolled case, the arc distributions remain Gaussian, providing a stable, symmetric heat flux and therefore uniform solidification. During the control experiment, the arc was localized to the outer perimeter, thus producing an asymmetric solidification profile.



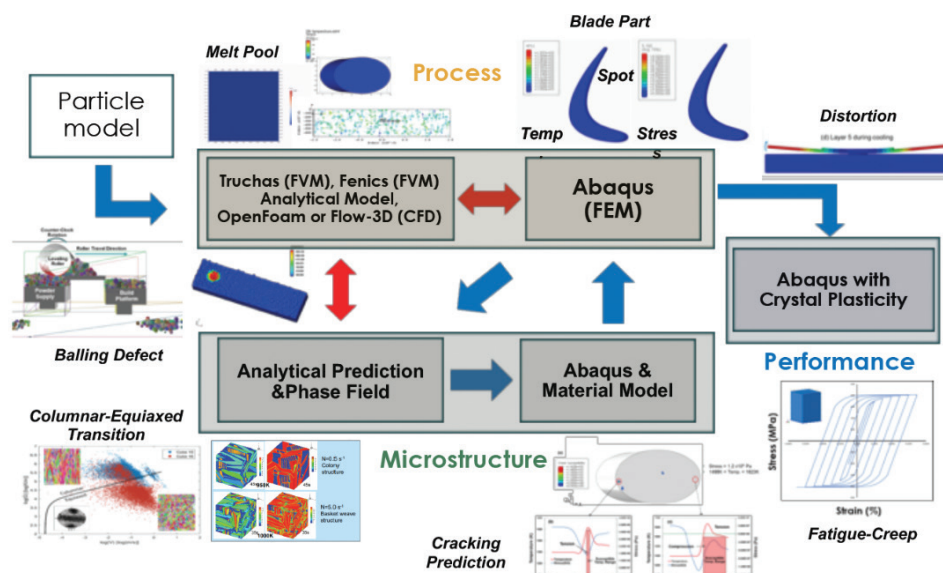
## Components Fabricated by Additive Manufacturing

<b>Performer</b>	Oak Ridge National Laboratory (ORNL)
<b>Award Number</b>	FWP-FEAA128
<b>Project Duration</b>	10/01/2018 – 09/30/2021
<b>Total Project Value</b>	\$ 900,000
<b>Collaborator</b>	Siemens
<b>Technology Area</b>	Plant Optimization Technologies

The goal of this project is to develop predictive tools to correlate additive manufacturing (AM) process parameters with bulk material properties of components using machine learning algorithms. There are several key challenges currently confronting AM processes for metal-based alloys. The internal microstructures, micro-, meso- and macro- (or part-) level physical properties, and performance under load are all dependent on the manufacturing process. The large number of AM processing parameters available means that AM manufacturing R&D can be very long and expensive if done without the use of process and materials modeling tools. With modeling, the various interactions and parameter sensitivities can be investigated independently of each other. For AM, where the understanding of the effects of feedstock properties, deposition rates, thermal history, cooling rates, phase transformation, defect formation, and

residual stress are still in an early phase, the framework to accurately predict the part properties is not well established.

Various physics-based models will be developed to describe all steps of the AM process, allowing the determination of the alloy microstructure and mechanical properties based on the AM process parameters. A machine learning approach will also be investigated to enable rapid qualification of high-temperature structural alloys with increased additive manufacturing process reliability, which will enable design flexibility for full utilization of additive manufacturing. Collaboration between ORNL and Siemens will provide a unique opportunity to develop a simulation process that connects the process parameters through modeling to part microstructure and bulk mechanical properties and to validate the process using test data on CM 247 and Haynes 282 alloys.



Model structure for prediction of AM process-microstructure-property correlations.

## Development of Functionally Graded Transition Joints to Enable Dissimilar Metal Welds

<b>Performer</b>	Oak Ridge National Laboratory (ORNL)
<b>Award Number</b>	FWP-FEAA151
<b>Project Duration</b>	07/01/2019 – 09/30/2021
<b>Total Project Value</b>	\$ 1,000,000
<b>Technology Area</b>	Plant Optimization Technologies

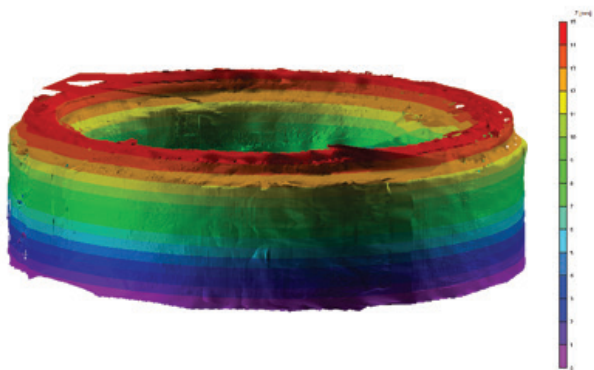
Oak Ridge National Laboratory will weld dissimilar metals using functionally graded transition joints that exhibit high resistance to creep and fatigue and high microstructural stability. The primary focus of the project will be on joining ferritic steels to austenitic steels, in particular alloys that are relevant in coal-fired power plants. A key aspect of the proposed 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

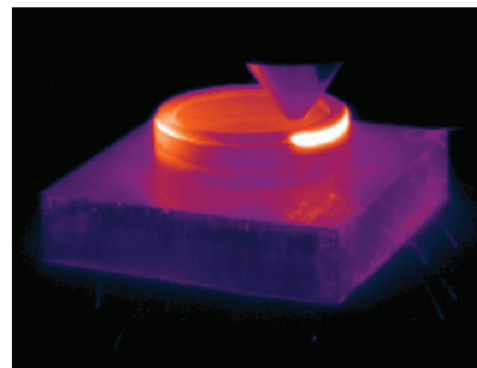
diffusion and the formation of stresses induced by thermal expansion mismatch.

- 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.



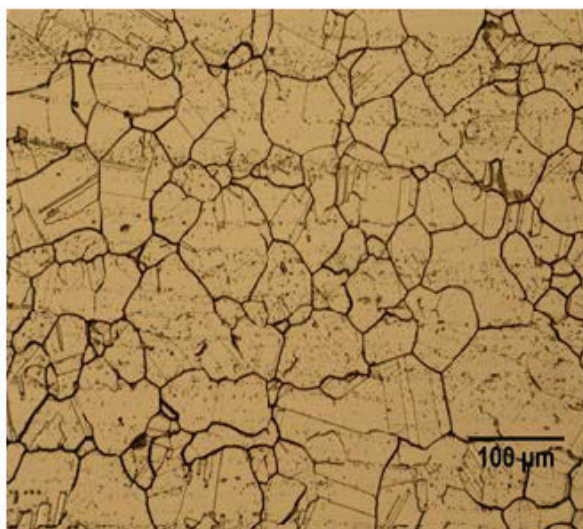
IR image showing temperature  
distribution with build height.

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

<b>Performer</b>	Pacific Northwest National Laboratory (PNNL)
<b>Award Number</b>	FWP-71843
<b>Project Duration</b>	10/01/2018 – 09/30/2021
<b>Total Project Value</b>	\$ 1,120,000
<b>Technology Area</b>	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 proposed 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<sub>2</sub> heat exchangers).



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



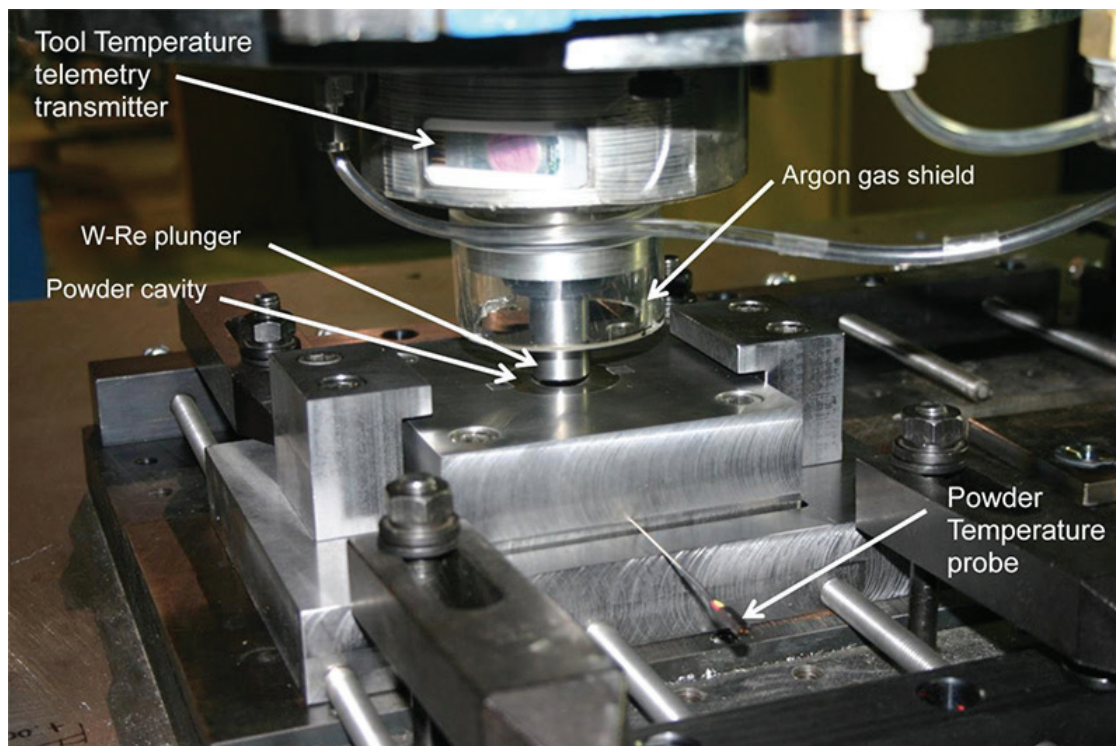
## Low Cost Fabrication of ODS Materials

<b>Performer</b>	Pacific Northwest National Laboratory (PNNL)
<b>Award Number</b>	FWP-60098
<b>Project Duration</b>	10/01/2010 – 09/30/2021
<b>Total Project Value</b>	\$ 735,000
<b>Technology Area</b>	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

<b>Performer</b>	Pacific Northwest National Laboratory (PNNL)
<b>Award Number</b>	FWP-66059
<b>Project Duration</b>	10/1/2014 – 9/30/2021
<b>Total Project Value</b>	\$ 1,075,000
<b>Technology Area</b>	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.

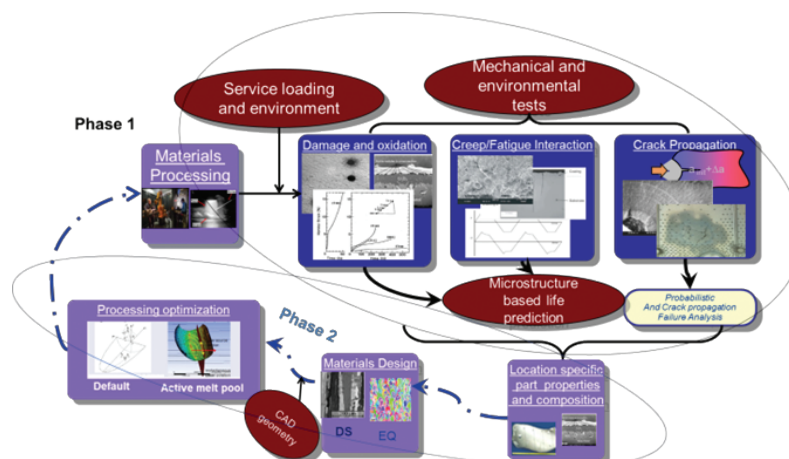
# Optimization of Wire Arc Additive Manufacturing (WAAM) Process to Produce Advanced Ultra-Supercritical Components (AUSC) Components with Increased Service Life

<b>Performer</b>	Raytheon Technologies
<b>Award Number</b>	FE0031821
<b>Project Duration</b>	10/01/2019 – 09/30/2021
<b>Total Project Value</b>	\$ 1,249,916
<b>Collaborator</b>	Siemens
<b>Technology Area</b>	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. The recipient 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 Ultra-Supercritical Power Plant

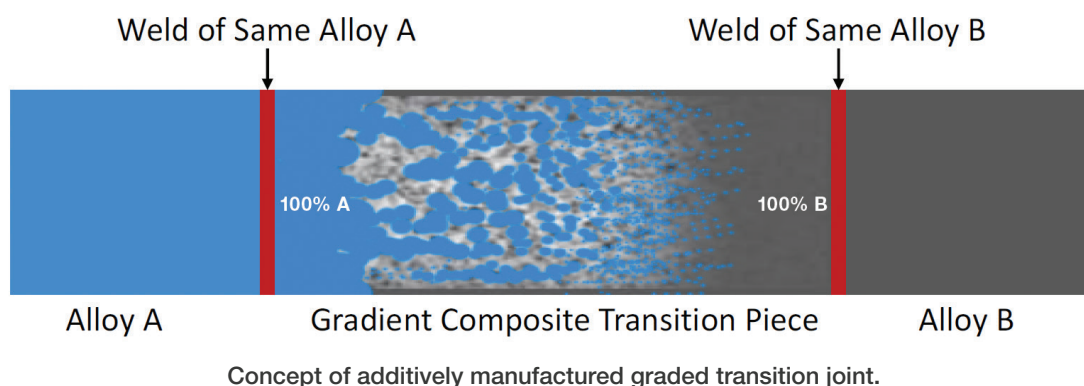
Performer	West Virginia University	Oak Ridge National Laboratory (ORNL)
Award Number	FE0031819	FWP-FEAA372
Project Duration	10/01/2019 – 03/31/2021	10/01/2019 – 09/30/2021
Total Project Value	\$ 959,865	\$ 310,000
Total Project Value (All)	\$ 1,269,865	
Collaborators	Carpenter Powder Products; General 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.





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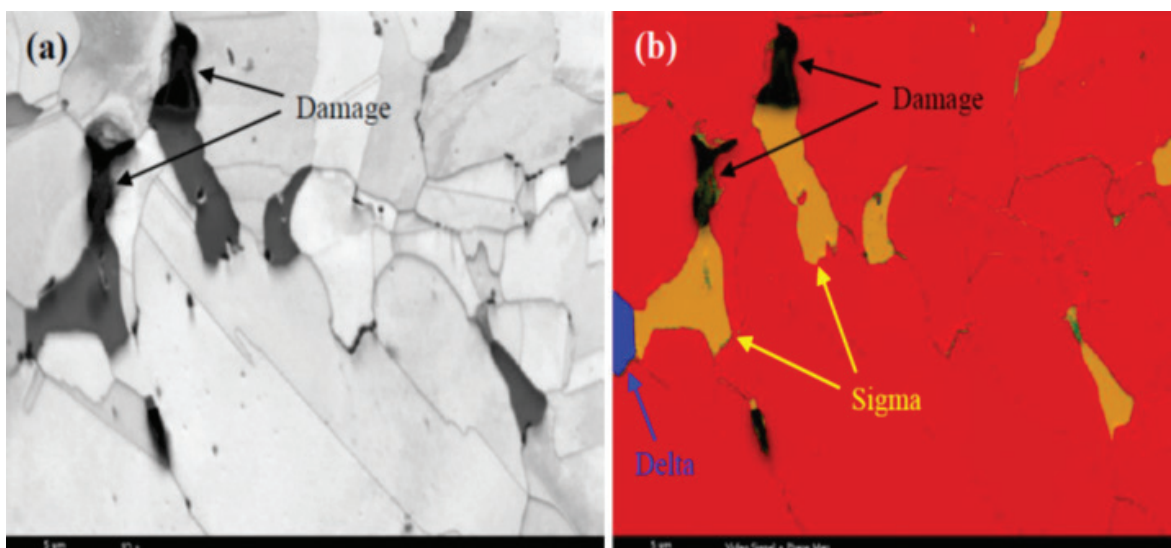
## Characterization of Long-Term Service Coal Combustion Power Plant Extreme Environment Materials (EEMs)

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

NETL is partnering 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.

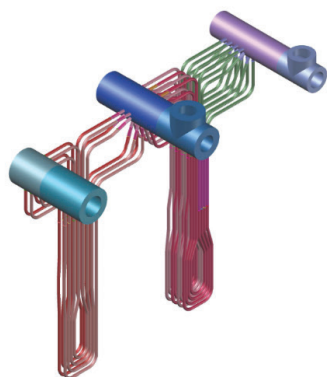
## Advanced Ultra-Supercritical Component Testing

<b>Performer</b>	Energy Industries of Ohio, Inc.
<b>Award Number</b>	FE0025064
<b>Project Duration</b>	11/01/2015 – 09/30/2021
<b>Total Project Value</b>	\$ 27,311,822
<b>Collaborators</b>	AECOM; Alstom Power, Inc.; Electric Power Research Institute, Inc.; GE Power and Water; MetalTek International; Riley Power; Special Metals; Thermal Engineering; Youngstown Thermal
<b>Technology Area</b>	Plant Optimization Technologies

The National Energy Technology Laboratory is partnering 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 °C (1400 degrees °F) 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

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

The recipient 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 nanostructured ferritic alloy (NFA) and an oxidation protective coating across the joint retrofittable in the existing fleet. These proposed 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.



## Advanced Alloy Development

<b>Performer</b>	National Energy Technology Laboratory (NETL)
<b>Award Number</b>	FWP-1022406
<b>Project Duration</b>	01/01/2017 – 03/31/2022
<b>Total Project Value</b>	\$ 10,718,127
<b>Technology Area</b>	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

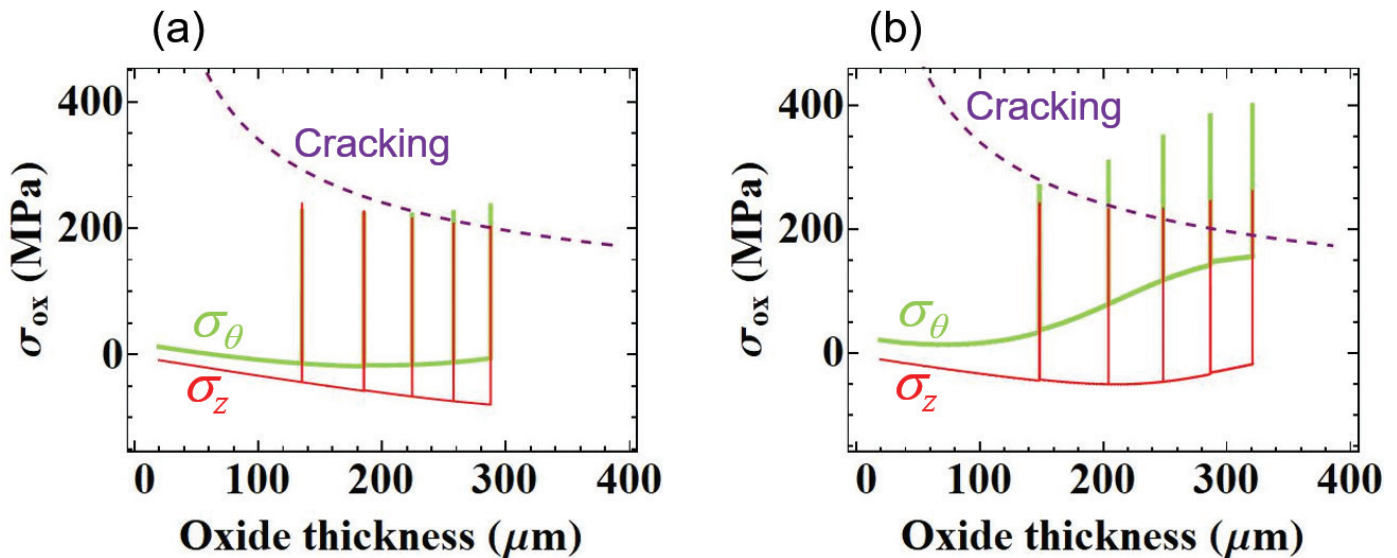
to guide and accelerate alloy design and manufacturing development.

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

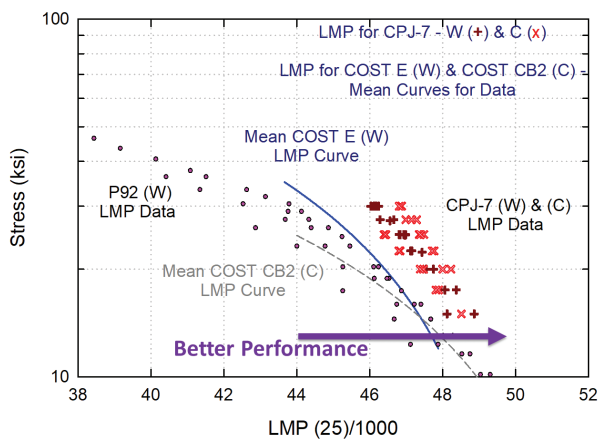
*Materials for sCO<sub>2</sub> Power Cycles: Alloy Performance*—Determine whether available AUSC power plant materials are suitable for fossil fuel supercritical carbon dioxide (sCO<sub>2</sub>) service in terms of temperature and stress, and if they are, assess the potential physical and mechanical consequences of their use.

*Materials for sCO<sub>2</sub> Power Cycles: Materials and Manufacturing Issues Associated with Heat Exchangers for sCO<sub>2</sub> 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<sub>2</sub> power cycles.

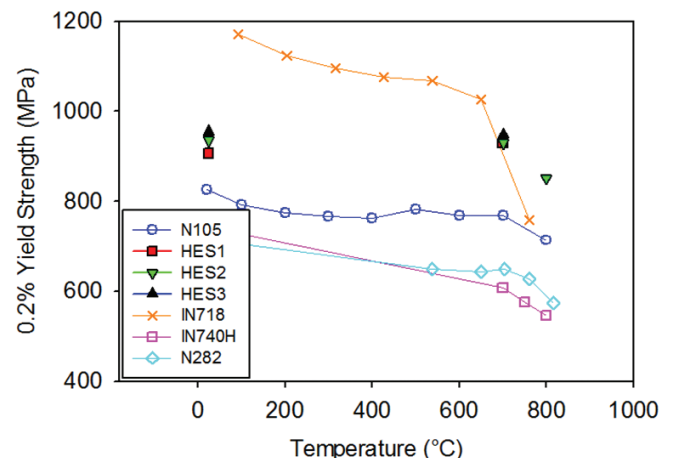
The structural materials and manufacturing processes researched in this FWP are needed to lower the cost and improve the performance of fossil-based power-generation. Additionally, the development and utilization of computational simulation and broad-based data analytic tools can further reduce the time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



Damage maps for T91 boiler tubes under (a) subcritical steam conditions and (b) supercritical steam conditions. The solid lines are calculated stresses from simulations (green lines: hoop stress; red lines: axial stress), while the dashed lines denote the critical stress for through-scale cracking. The spikes of the solid lines are caused by the extra thermal stress during shut-down events.



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



Using high entropy alloy design concepts, NETL designed more stable gamma prime strengthened superalloys (yield strength of NETL high entropy superalloys (HES1, HES2, and HES3) compared to conventional superalloys).

## Corrosion Issues in Advanced Coal Fired Boilers

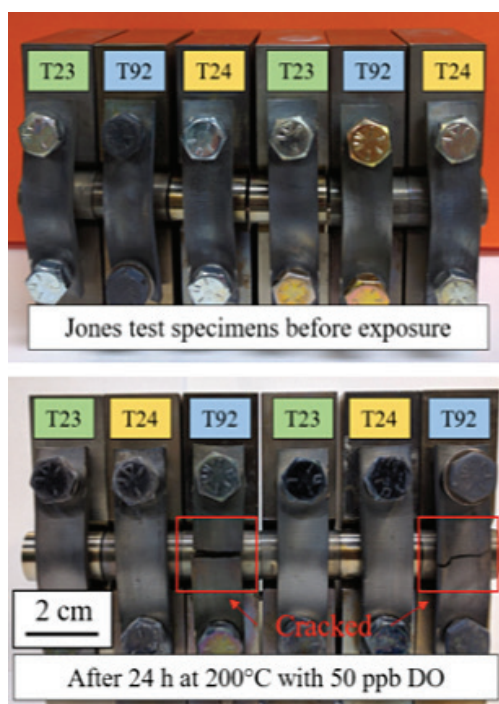
<b>Performer</b>	Oak Ridge National Laboratory
<b>Award Number</b>	FWP-FEAA116
<b>Project Duration</b>	10/1/2013 – 06/30/2021
<b>Total Project Value</b>	\$ 1,764,250
<b>Technology Area</b>	Plant Optimization Technologies

NETL is partnering with ORNL to address critical corrosion and environmental effects issues in coal-fired boilers ranging from boiler water walls to superheater tubes. Specific technical objectives are to get a better understanding of (1) hydrogen-induced cracking in boiler water walls and which alloys may be more resistant to this type of degradation, and (2) the effect of shot peening on steamside oxidation of austenitic superheater tubes. Such knowledge is critical to efforts to develop more accurate lifetime prediction models for current alloys used in boilers and advanced alloys and surface modifications that are being considered for use in

advanced coal-fired power systems.

The project goal will be achieved by determining the temperature-relevant corrosion mechanisms, determining the role of environment on mechanical response, evaluating the upper temperature limit for new materials and surface modifications in terms of lifetime, and characterizing the reaction products and extent of alloy degradation under these conditions.

The results should improve performance of commercial and model alloys in controlled laboratory experiments to simulate advanced fossil boiler conditions.



Jones tests with controlled water chemistry.

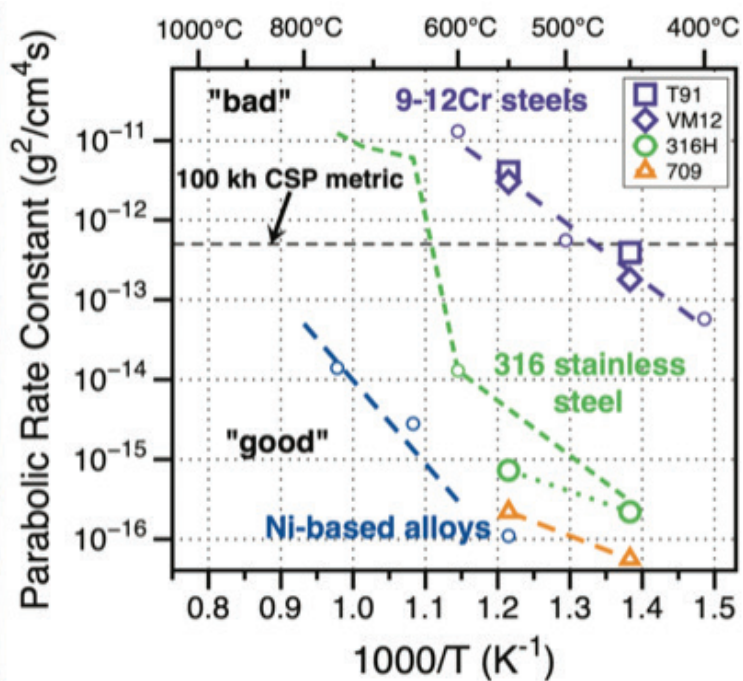
## Effect of Impurities on Supercritical Carbon Dioxide Compatibility

<b>Performer</b>	Oak Ridge National Laboratory (ORNL)
<b>Award Number</b>	FWP-FEAA144
<b>Project Duration</b>	10/01/2019 – 05/31/2022
<b>Total Project Value</b>	\$ 1,650,000
<b>Technology Area</b>	Plant Optimization Technologies

The proposed work will study the effect of impurities (e.g., O<sub>2</sub>; H<sub>2</sub>O) on compatibility of structural materials in supercritical carbon dioxide (sCO<sub>2</sub>) Brayton cycle systems, particularly for direct-fired systems. High impurity levels (0.25–1 percent) have been found to increase reaction rates of both Fe- and Ni-based alloys at 750 degrees °C/300 bar (30 megapascals; MPa). Further work is needed to isolate O<sub>2</sub> and H<sub>2</sub>O effects including the use of isotopic tracers and to understand creep behavior of thin-walled sections for Fe- and Ni-based alloy heat exchangers. 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 as methods 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.

The purpose of this project is to continue laboratory testing with the goal of further understanding the role of impurities on structural alloy compatibility in sCO<sub>2</sub> in order to support the design and development of economical commercial systems. Using unique experimental equipment developed under the previous project, a more detailed understanding of the effect of gas impurities on sCO<sub>2</sub> compatibility in direct-fired cycles will be explored at 750 °C/300 bar. In addition, creep testing of thin-sectioned Fe- and Ni-based alloys will determine if creep properties are altered in thin-sections and degraded by oxidation. The impact of impurities on sCO<sub>2</sub> compatibility also will be explored for Fe-based alloys at lower temperatures (450°–650 °C) to determine maximum use temperatures for 9–12%Cr and austenitic steels. In addition to evaluating reaction rates and characterizing reaction products, compatibility also will be assessed by measuring post-exposure room temperature tensile properties, which also reflect alloy degradation. Interactions with industry will continue to identify impurity levels of interest and critical materials issues for future investigations. A further objective is to communicate the generated information to the sCO<sub>2</sub> community and materials suppliers, as well as to the high-temperature materials community in general, as appropriate.





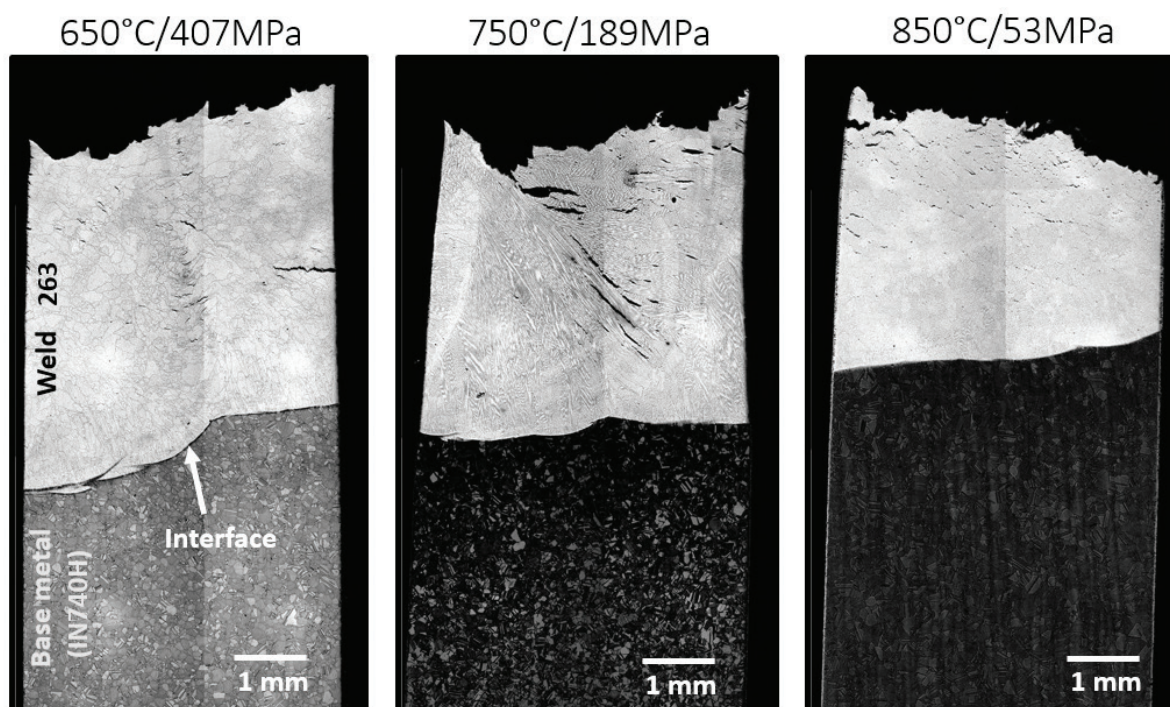
ORNL is evaluating structural steels at 450°–650°C in 30MPa supercritical  $\text{CO}_2$  using laboratory autoclaves (left) to determine under what conditions the reaction rates are low enough for power generation applications. On the right, an Arrhenius plot of parabolic rate constants compares rate constants measured on this project to literature values.

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

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

The objective of this project is to evaluate 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 °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 insights into potential manufacturability issues related to large-scale components made from Ni-based alloys and 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.

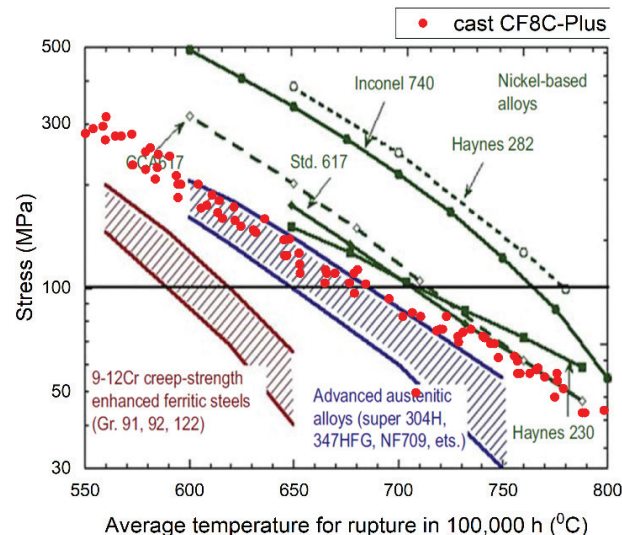
## Low Cost High Performance Austenitic Stainless Steels for A-USC

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

The objective of this project is to evaluate 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 particularly focused on obtaining long-term creep properties of full- or near-full-sized components of extruded tubes and pipes or otherwise 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

<b>Performer</b>	Oak Ridge National Laboratory (ORNL)
<b>Award Number</b>	FWP-FEAA137
<b>Project Duration</b>	10/01/2018 – 09/30/2021
<b>Total Project Value</b>	\$ 900,000
<b>Technology Area</b>	Plant Optimization Technologies

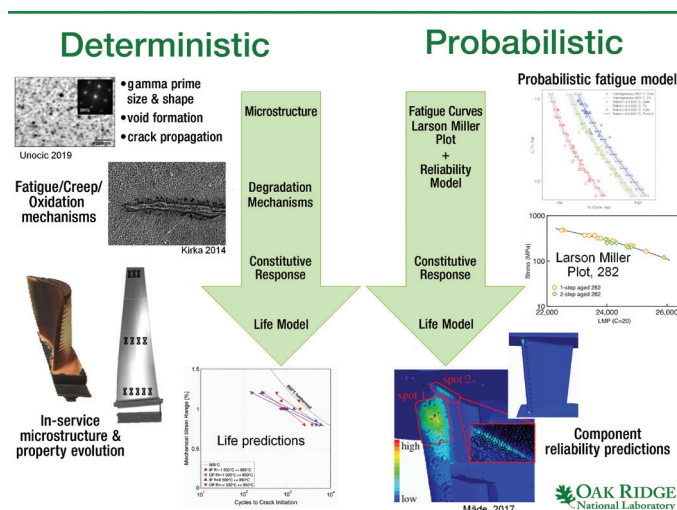
The goal of this project is to improve lifetime model prediction for nickel-based superalloy power plant components. The microstructure and properties of parts exposed in the field for up to 32,000 hours will be characterized to determine the evolution of key lifetime damage parameters. Synergy between 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

<b>Performer</b>	Oak Ridge National Laboratory (ORNL)
<b>Award Number</b>	FWP-FEAA150
<b>Project Duration</b>	08/01/2019 – 09/30/2022
<b>Total Project Value</b>	\$ 900,000
<b>Technology Area</b>	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

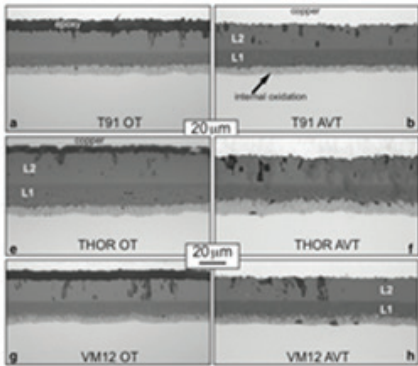
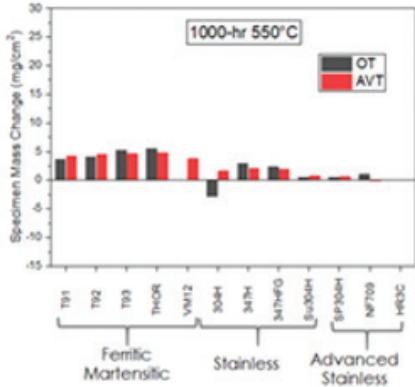
quantitative analysis of the adhesion and exfoliation behavior of both ferritic and austenitic steels. A better understanding of the underlying mechanisms will allow a realistic lifetime prediction of currently employed materials under a range of partial- and full-load duty cycles and suggest avenues for the deployment of surface modifications including coatings and shot peening.

## Testing



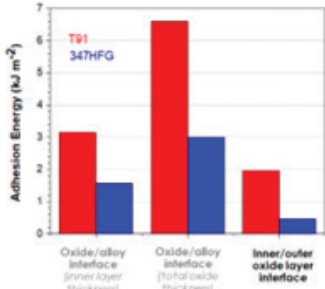
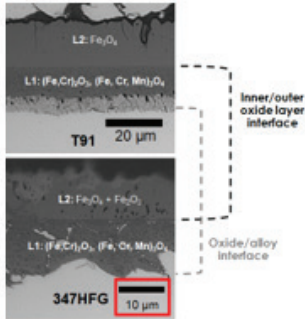
- 275 bar water, 50-h cycles, 550-650°C
- Ferritic-martensitic and austenitic steels
- **Controlled water chemistry:**  
OT (100ppb O<sub>2</sub>),  
AVT (<10 ppb O<sub>2</sub>)
- **Additions:** 2 film forming products (amines)

## 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 corresponds well to observed failure interface

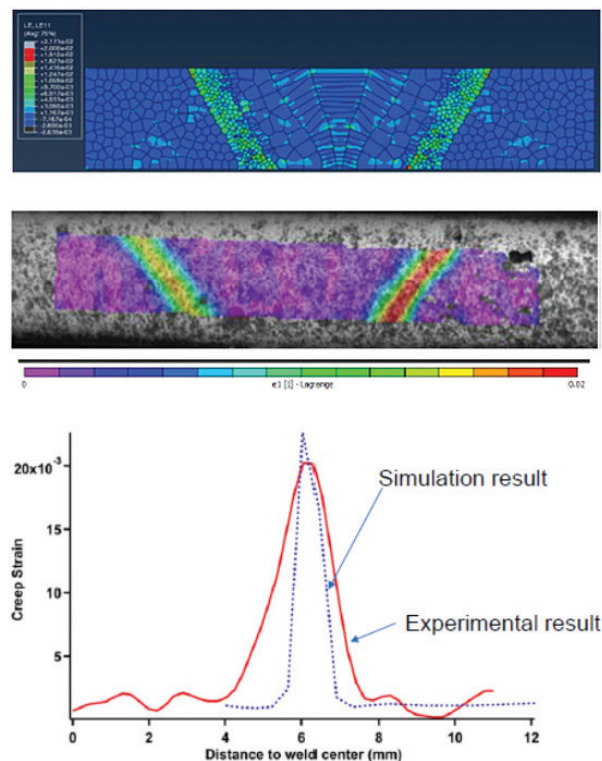
## Weldability of Creep Resistant Alloys for Advanced Power Plants

<b>Performer</b>	Oak Ridge National Laboratory (ORNL)
<b>Award Number</b>	FWP-FEAA118
<b>Project Duration</b>	10/01/2013 – 09/30/2021
<b>Total Project Value</b>	\$ 1,800,000
<b>Technology Area</b>	Plant Optimization Technologies

NETL is partnering 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 work 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.

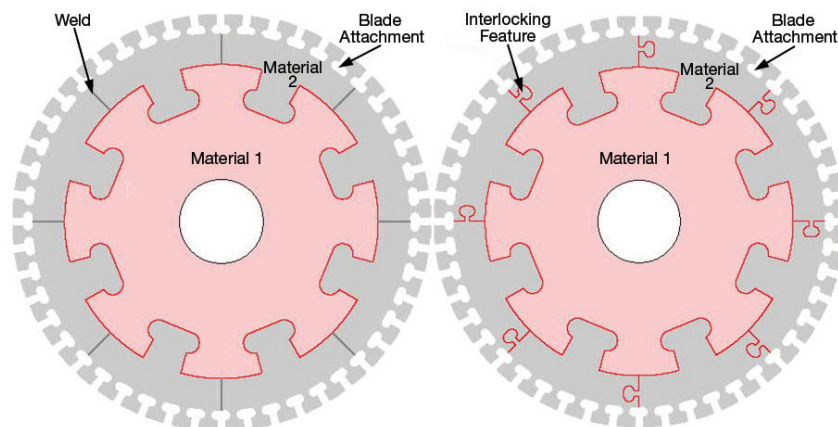
## Welding of Haynes 282 to Steels to Enable Modular Rotors for Advanced Ultra Super-Critical Steam Turbines

<b>Performer</b>	Siemens Corporation
<b>Award Number</b>	FE0031824
<b>Project Duration</b>	10/01/2019 – 08/31/2021
<b>Total Project Value</b>	\$ 1,408,866
<b>Technology Area</b>	Plant Optimization Technologies

This project will weld Haynes 282 (H282) superalloy plates and/or rounds (up to 3 inches thick) to similarly shaped grades of common rotor steels (3.5NiCrMoV steel and 9-12%Cr steel). The work involves developing weld designs that seek to minimize residual stresses, distortion, and weld defects when H282 is welded to steels. Simulation software will be used to simulate multiple weld designs to downselect the most promising ones. Simulation-derived designs will be used to make actual welds to further refine the weld parameters. Successful welds will be examined ultrasonically using the synthetic aperture focusing technique (SAFT). Welded test pieces incorporating H282 will be machined using automated spindle-speed adjustment to enhance tool life. A data-driven digital twin of tool flank wear evolution in a longitudinal turning operation will be created on a cloud platform. The data will be used to train a Gaussian process regression (GPR) model to predict the average tool flank wear as a function of the measured quantities. A web application running the GPR model on the cloud platform will be used to forecast the remaining tool life during turning operations

and adjust the spindle speed to automatically extend tool life by the desired amount. The scope of this project is geared towards answering the questions that would allow a steam turbine rotor to be made that is suitable for advanced ultrasupercritical (AUSC) applications in coal-fired power plants from 100 megawatt electrical to 1 gigawatt electrical size, and service conditions of at least 760 °C and 3,100 pounds per square inch absolute pressure.

The technology developed here will enable the manufacturing of welded rotors (welding H282 to steels) for steam turbines for AUSC applications. Modular construction of rotors using smaller forgings of superalloys only in locations where needed is thus enabled. By using superalloys in selected areas of the rotor, the rotor will withstand significantly higher temperatures, such as those encountered in AUSC cycles. The successful completion of this technology development is expected to enable AUSC fossil-fired powerplants to be more economical and technically viable and thus to play their necessary and important role in the transition of the United States towards a balanced energy portfolio.



Configuration of different materials welded together to form a hybrid rotor.

## Development of Corrosion- and Erosion-Resistant Coatings for Advanced Ultra-Supercritical Materials

<b>Performer</b>	Tennessee Technological University
<b>Award Number</b>	FE0031820
<b>Project Duration</b>	10/01/2019 – 09/30/2021
<b>Total Project Value</b>	\$ 1,030,754
<b>Collaborators</b>	Eastern Plating; Oak Ridge National Laboratory; Purdue University; Siemens
<b>Technology Area</b>	Plant Optimization Technologies

Tennessee Technological University (TTU), in coordination with Purdue University, Oak Ridge National Laboratory, Siemens Corporation, and Eastern Plating, will develop and evaluate corrosion- and erosion-resistant coatings for advanced ultrasupercritical (AUSC) materials using a cost-effective electrolytic codeposition process. The goal is to enhance both corrosion and erosion properties of the electro-codeposited coatings for the protection of high-pressure (HP) steam turbine blades in AUSC pulverized coal fired power plants that will operate at temperatures and pressures up to 760 °C (1400 °F) and 35 MPa (5000 psi).

To expedite coating development, the team will initially execute a computational design effort to guide selection of coating chemistry and optimization of processing parameters. In addition to commercial Ni-base alloys, TTU will explore electro-codeposited coatings on the alloys made

by additive manufacturing. Electro-codeposition, a process in which fine powders dispersed in a plating solution are codeposited with the metal onto the substrate to form a composite coating, provides a versatile and convenient route to the realization of a wide range of coatings, such as metal matrix composites containing hard ceramic particles (e.g., silicon carbide or tungsten carbide) to improve the wear resistance of the rotor tips and the piston internal cylinder surfaces of automotive engines. Based on the findings of the previous AUSC Materials Consortium's study, a composition similar to Tribaloy T400-C will be used as the baseline coating. If successful, this project will result in cost-effective coating solutions that enhance the durability of AUSC turbine materials with respect to corrosion and erosion for increased power generation efficiency, and/or to provide existing FE power plants extended life.

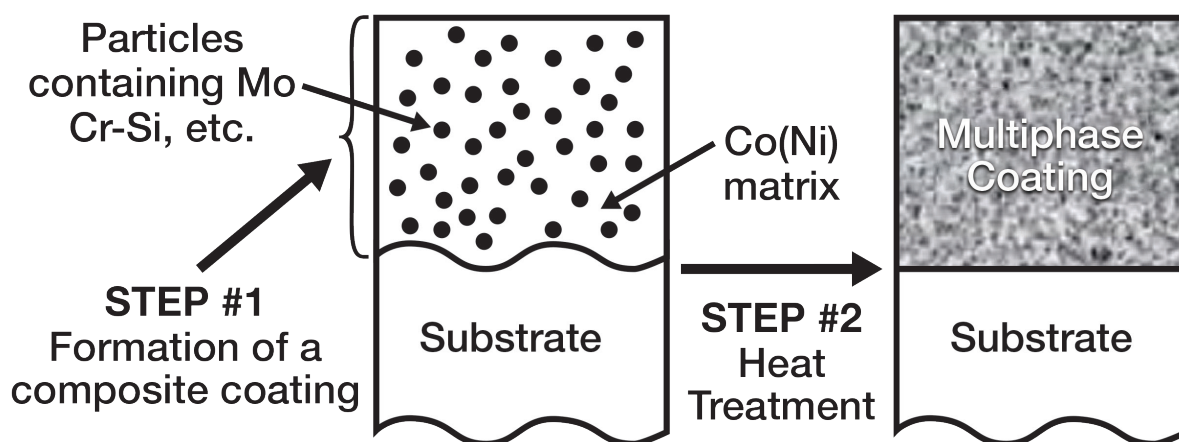


Illustration of the electro-codeposition coating process.



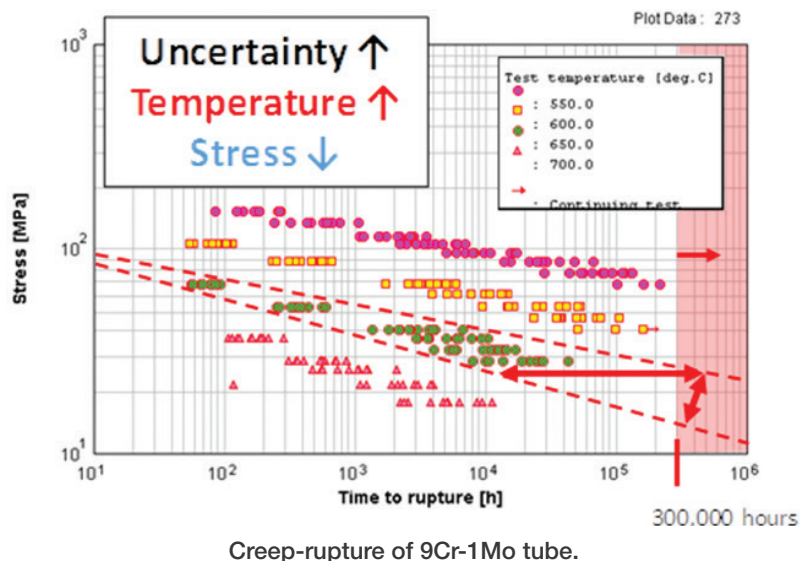
# An Accelerated Creep Testing Program for Advanced Creep Resistant Alloys for High Temperature Fossil Energy Applications

<b>Performer</b>	University of Texas at El Paso
<b>Award Number</b>	FE0030331
<b>Project Duration</b>	09/01/2017 – 02/28/2021
<b>Total Project Value</b>	\$ 400,000
<b>Technology Area</b>	University Training and Research

NETL is partnering with the University of Texas at El Paso to vet, improve, and test the feasibility of accelerated creep testing (ACT) for metallic materials. These overarching goals will be achieved by the following technical approach. A database of long-term creep data for surrogate materials P91 steel and Inconel 718 nickel-based superalloy will be collected. Pre-ACT experiments will be performed to establish the baseline properties of the material, evaluate a reference-calibration approach for the ACTs, and develop a creep deformation mechanisms map. The framework of the ACTs will be scrutinized, and mathematical rules and constraints posed to establish the systematic repeatability of time acceleration. A targeted test matrix of ACTs will be executed to probe the limits of time acceleration. A post-audit validation where ACT tests are compared to the experimental database will be used to determine the extent

to which the ACTs are independent of systematic errors and calibration bias. Finally, a comprehensive standardized “Test Standard – An Accelerated Creep Testing Program for New Material Qualification” will be written that includes geometry, test parameters, regression software, and recommendations for the retrofit of existing creep frames.

This project has the potential to reduce the time to implementation of new creep-resistant alloys from decades to months. The ACTs could enable the collection of multistage creep deformation and rupture of extremely long-lived ( $10^6$  hours) metallic materials in less than 24 hours. The outcome of this study will be an accelerated creep testing program for new material qualification. Original equipment manufacturers and plant owners can then use this knowledge to design and predict the remaining life of fossil energy components with more reliability.



## COMPUTATIONAL MATERIALS DESIGN

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## eXtremeMAT: Extreme Environment Materials

Performer	National Energy Technology Laboratory	Ames National Laboratory	Idaho National Laboratory	Lawrence Livermore National Laboratory	Los Alamos National Laboratory	Oak Ridge National Laboratory	Pacific Northwest National Laboratory
Award Number	FWP-1022433	FWP-AL-17-510-091	FWP-B000-17016	FWP-FEW0234	FWP-FE-850-17-FY17	FWP-FEAA134	FWP-71133
Project Duration	10/01/2018 – 09/30/2021	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020
Total Project Value	\$ 2,065,645	\$ 981,000	\$ 628,000	\$ 590,000	\$ 2,063,000	\$ 1,604,000	\$ 1,090,000
Total Project Value (All)	\$ 9,021,645						
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<sub>2</sub>) 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 brings 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

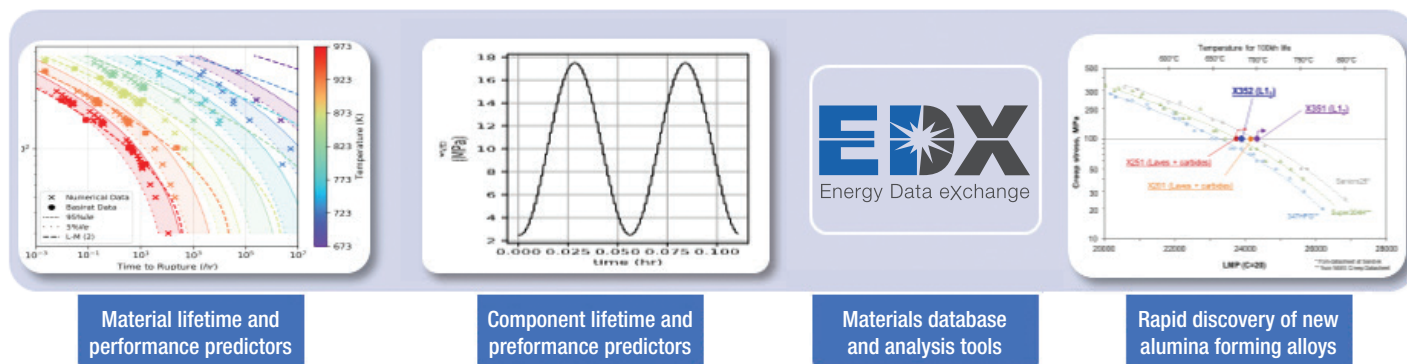
energy applications. In addition, materials modeling and life prediction and the models developed therein can be used to assess the current and remaining life integrity of heat-resistant alloys used in existing plants. It may also be possible to improve the performance envelope of current-generation fossil energy alloys by understanding the relationship between manufacturing, microstructural stability, and mechanical behavior.

Initially, the effort will target enabling sCO<sub>2</sub> 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<sub>2</sub> 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 °C, 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<sub>2</sub> 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.

For more information visit the eXtremeMAT website at: <https://edx.netl.doe.gov/extrememat/>





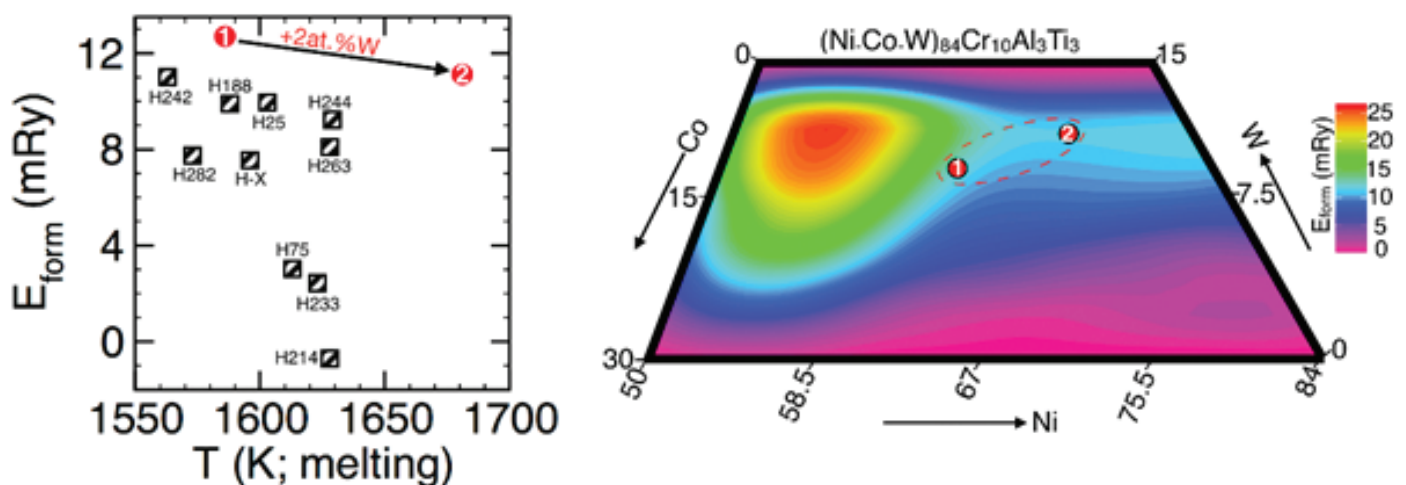
## Predictive Design of Novel Ni-based Alloys

<b>Performer</b>	Ames National Laboratory
<b>Award Number</b>	FWP-AL-19-510-097
<b>Project Duration</b>	04/08/2019 – 09/30/2021
<b>Total Project Value</b>	\$ 750,000
<b>Technology Area</b>	Plant Optimization Technologies

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

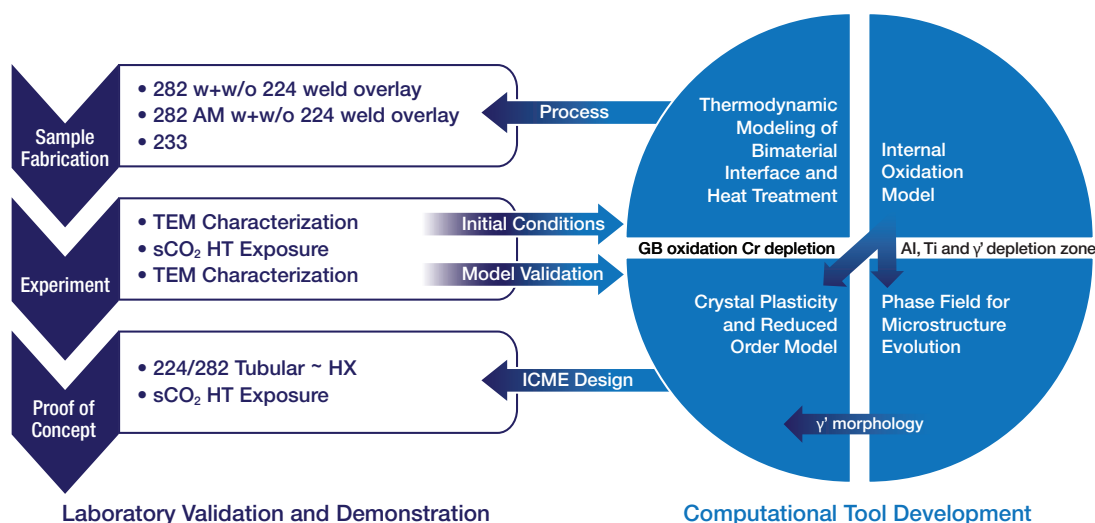
## ICME for Advanced Manufacturing of Nickel Superalloy Heat Exchangers with High Temperature Creep Plus Oxidation Resistance for Supercritical CO<sub>2</sub>

<b>Performer</b>	Det Norske Veritas (DNV) GL USA, Inc.
<b>Award Number</b>	FE0031631
<b>Project Duration</b>	10/01/2018 – 09/30/2021
<b>Total Project Value</b>	\$ 937,500
<b>Collaborator</b>	Ohio State University
<b>Technology Area</b>	Coal Utilization Science

Det Norske Veritas (DNV) GL USA will develop and validate computational design and analysis tools that optimize novel material combinations for fabricating microchannel heat exchangers via additive manufacturing for supercritical CO<sub>2</sub> power cycle technology. Original experiments will be performed for alumina and chromia scale-forming nickel-based superalloys made with conventional and additive manufacturing with simulated compositional grading effects. The project integrates high-temperature oxidation modeling, phase-field modeling of microstructure evolution, and creep performance using crystal plasticity modeling. The three models will be coupled according to an input-output matrix that passes information on solute depletion

into microstructure models for gamma-prime (γ') re-distribution and then into the crystal plasticity models for prediction of creep rate and tensile strength reduction. The modeling work will be tightly coupled with experimental high-temperature oxidation and creep testing of advanced alloys and prototype components in supercritical CO<sub>2</sub>.

This project could provide the fossil energy industry with new options for materials with property gradients. The integrated computational materials engineering (ICME) approach could improve pre-screening of fabrication techniques and heat treatments, which could reduce design time for materials intended for service in extreme environments.



Computational tool development pathway to support multi-material additive manufacturing for high-temperature heat exchange systems.

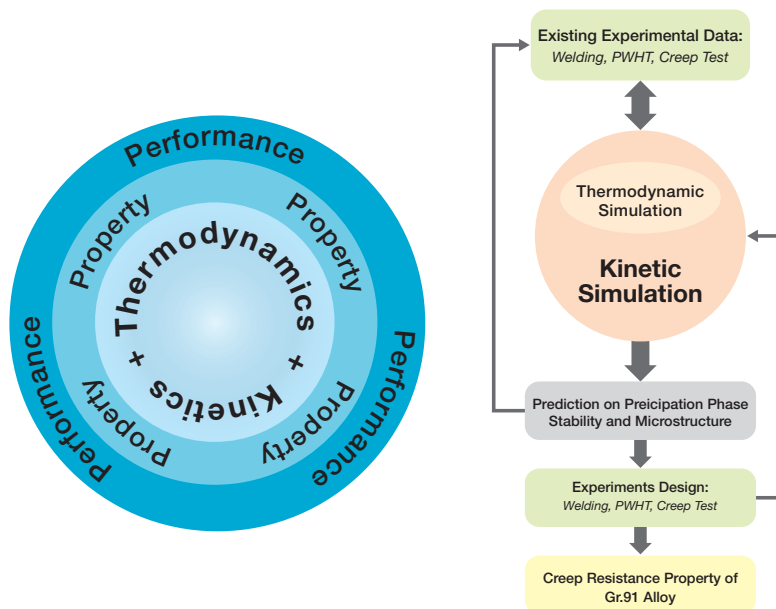
# The Fundamental Creep Behavior Model of Gr.91 Alloy by Integrated Computational Materials Engineering (ICME) Approach

<b>Performer</b>	Florida International University
<b>Award Number</b>	FE0027800
<b>Project Duration</b>	08/01/2016 – 01/31/2021
<b>Total Project Value</b>	\$ 250,000
<b>Collaborator</b>	Ohio State University
<b>Technology Area</b>	University Training and Research

NETL is partnering with Florida International University to investigate the fundamental creep cracking mechanism of the Grade 91 alloy under advanced power generation operating conditions to establish links among composition, processing parameters, phase stability, microstructure, and creep resistance using the ICME approach. Specifically, the project team will predict the phase stability and microstructure of Grade 91 base alloy and weldment with the computational thermodynamics and kinetics—calculation of phase diagrams (CALPHAD) approach; perform welding,

heat treatment, and creep testing of the Grade 91 alloy; develop a model that will provide an excellent match with experimental data from current and previous work on Grade 91 alloy; and predict how to improve the long-term creep resistance for the Grade 91 family of alloys.

The model will improve the creep resistance of Grade 91 alloys for use in advanced fossil-fueled power generation systems and other applications, thus increasing fossil-fueled power generation efficiency and reducing emissions.



Materials design using ICME approach.

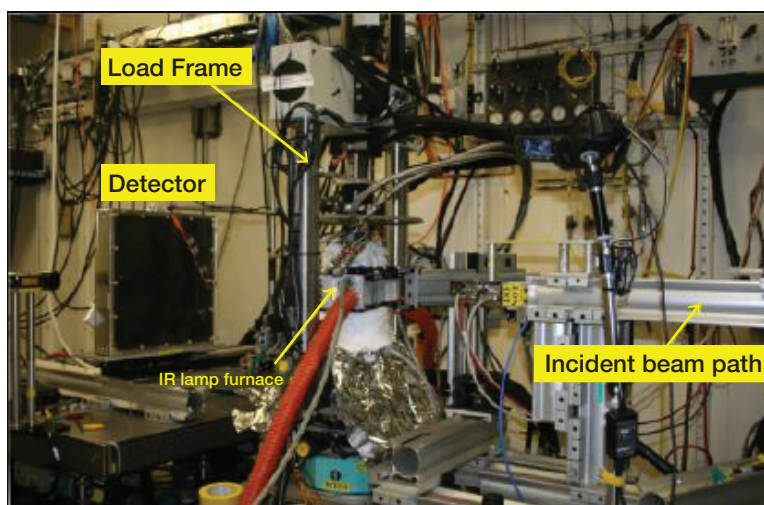
## Damage Accumulations Predictions for Boiler Components Via Macrostructurally Informed Material Models

<b>Performer</b>	General Electric (GE) Company
<b>Award Number</b>	FE0031823
<b>Project Duration</b>	10/01/2019 – 09/30/2022
<b>Total Project Value</b>	\$ 907,084
<b>Total Project Value</b>	\$ 937,084
<b>Collaborator</b>	Energy Industries of Ohio
<b>Technology Area</b>	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 °F. 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.



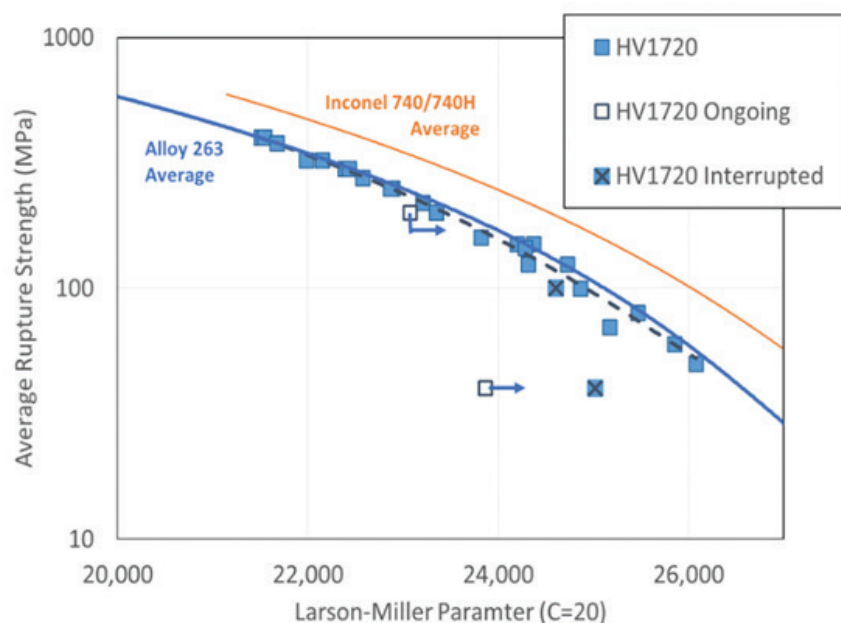
## Development of a Physically-Based Creep Model Incorporating ETA Phase Evolution for Nickel-Base Superalloys

<b>Performer</b>	Michigan Technological University
<b>Award Number</b>	FE0027822
<b>Project Duration</b>	08/15/2016 – 02/14/2021
<b>Total Project Value</b>	\$ 399,996
<b>Technology Area</b>	University Training and Research

NETL is partnering with the Michigan Technological University to develop a physically based creep model for Nimonic 263 that synthesizes known creep behavior based on gamma prime ( $\gamma'$ ) strengthening to gain a new understanding of the effects of eta phase on creep performance at long service times in fossil energy power plants. This project team will develop heat treatments for commercial Nimonic 263 to obtain a mixture of both eta ( $\eta$ ) and gamma prime phases prior to creep testing, with the  $\gamma'$  distribution being as close to commercial Nimonic 263 as possible; conduct creep tests on these materials at the Electric Power Research Institute; fully characterize

microstructures and deformation mechanisms during creep for all three alloys (standard Nimonic 263, Nimonic 263 heat-treated to contain  $\eta + \gamma'$ , and the Michigan Tech-modified Nimonic 263 alloy that contains only  $\eta$ ); and use the knowledge gained to develop and validate a physically-based creep model that synthesizes known gamma prime creep behavior to gain a new understanding of the effects of eta phase on creep performance.

The results will enhance life prediction, component design, and alloy selection for advanced fossil energy power plant systems.



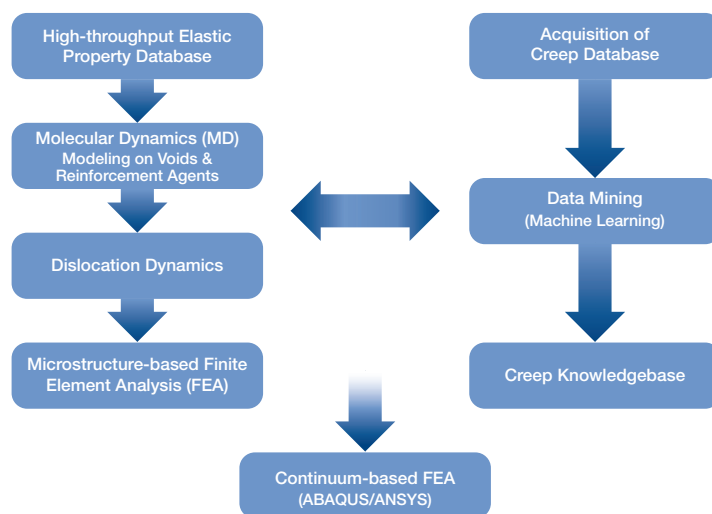
Alloy 20, Widmanstätten microstructure, creep.

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

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

NETL is partnering 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 proposed new roadmap to integrate the use of experimental creep database (“top-down” approach) with multi-scale modeling (“bottom-up” approach).

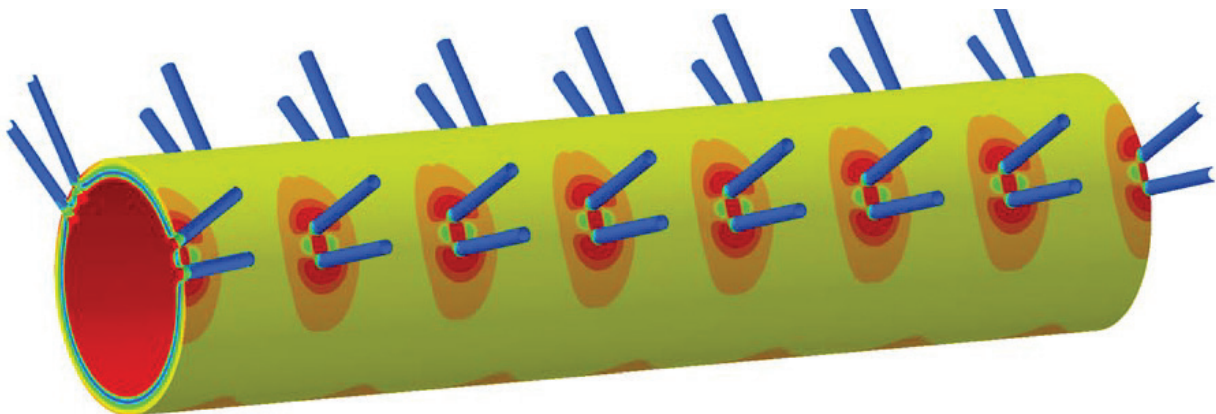
## Alloy for Enhancement of Operational Flexibility of Power Plants

<b>Performer</b>	North Carolina Agricultural and Technical State University
<b>Award Number</b>	FE0031747
<b>Project Duration</b>	08/15/2019 – 08/14/2022
<b>Total Project Value</b>	\$ 400,000
<b>Collaborator</b>	University of North Carolina Charlotte
<b>Technology Area</b>	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 the 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.



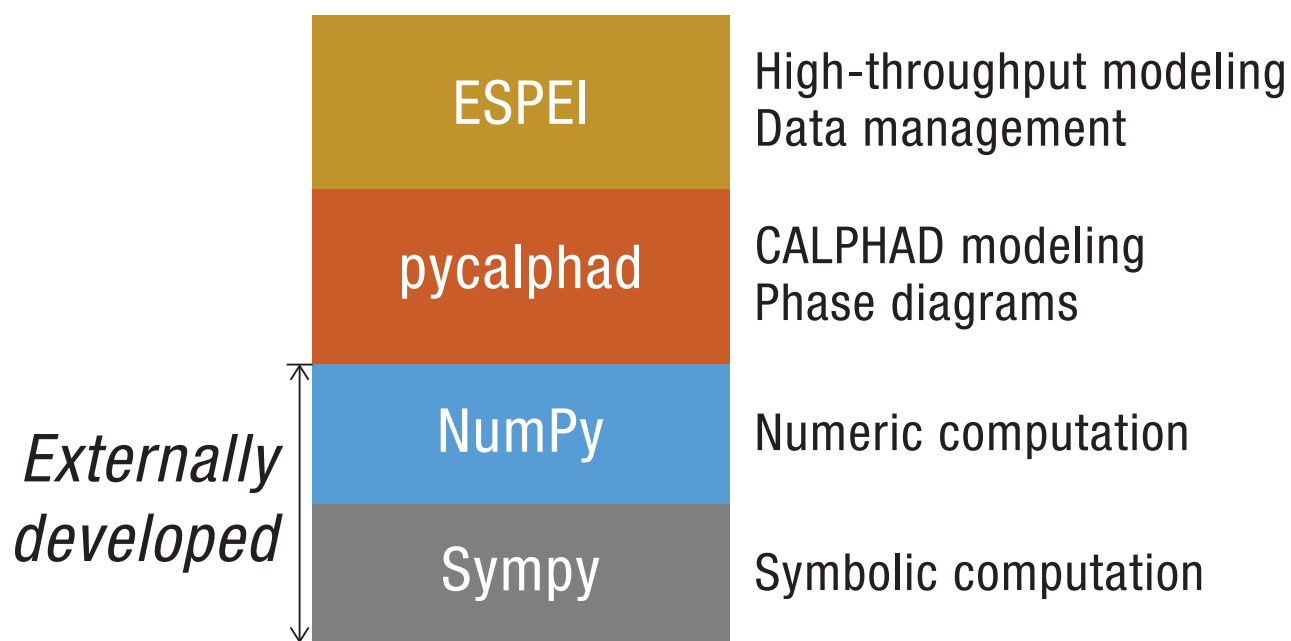
Stress contour plot of a steam header.

## High Throughput Computational Framework of Materials Properties for Extreme Environments

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

NETL is partnering 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 will be 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

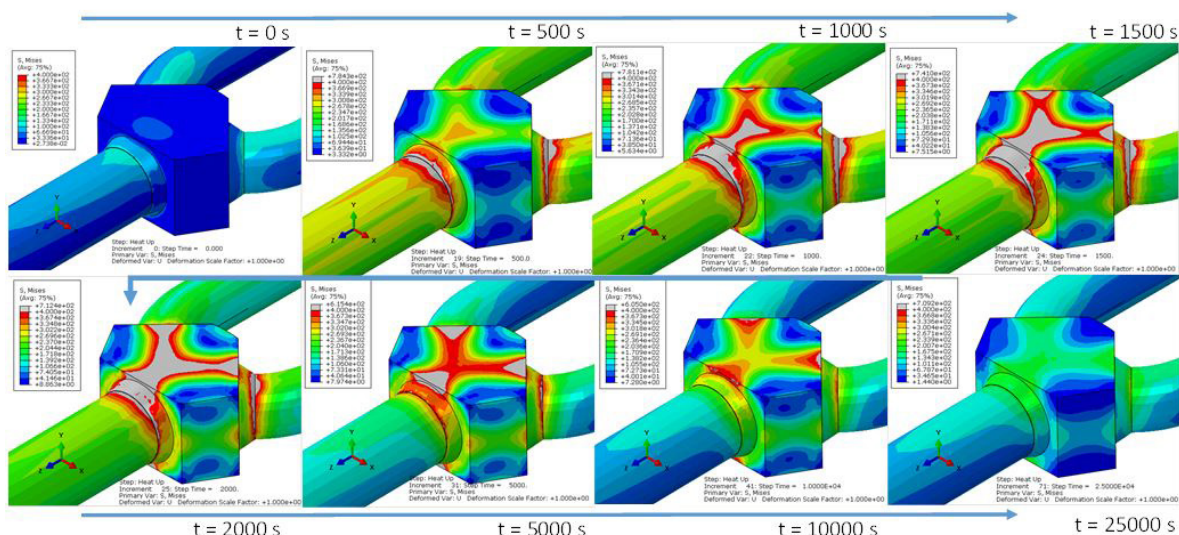
<b>Performer</b>	Southern Research Institute
<b>Award Number</b>	FE0031811
<b>Project Duration</b>	10/01/2019 – 09/30/2022
<b>Total Project Value</b>	\$ 862,345
<b>Technology Area</b>	Coal Utilization Science

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.

## Stress vs time



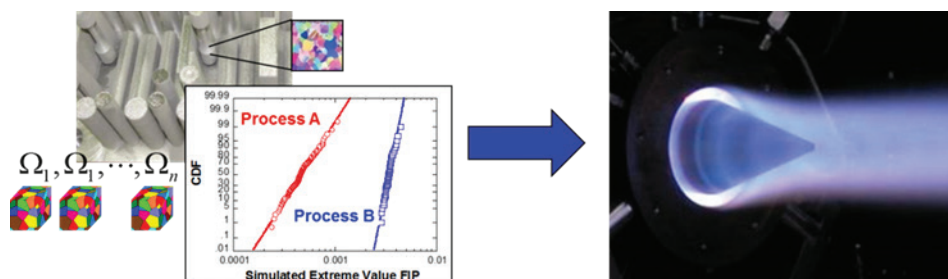
## Digital Twin Model for Advanced Manufacture of a Rotating Detonation Engine Injector

<b>Performer</b>	Southwest Research Institute (SwRI)
<b>Award Number</b>	FE0031644
<b>Project Duration</b>	10/01/2018 – 09/30/2021
<b>Total Project Value</b>	\$ 937,371
<b>Collaborators</b>	Aerojet Rocketdyne, Inc.; Georgia Tech Research Corporation
<b>Technology Area</b>	Coal Utilization Science

Southwest Research Institute (SwRI) will use a digital twin material model (DTMM) to apply advanced manufacturing techniques to advance rotating detonation engine (RDE) injector design. The project will develop both a digital twin model of the injector manufacturing process and an injector that performs in an RDE combustor with a significant reduction in flow loss. This will be accomplished through several subordinate objectives: design of a novel RDE injector that allows for fuel and oxidizer flows to be optimized in ways not possible with conventional manufacturing; comprehensive design of experiments (DofE) focusing on contributing factors that trigger high-cycle fatigue; development of a parametric material model based on actual test coupons from the advanced manufacturing process that allows prediction of mechanical strength properties; and manufacture, test, and post-test destructive evaluation of an RDE injector exposed to a significant high cycle fatigue environment. SwRI is responsible for the material model DofE, producing a portion of the material samples; performing the detailed RDE injector design; performance testing of the RDE injector; and post-test analysis of the injector component. Aerojet Rocketdyne will support the application of this work to the existing RDE;

review the DofE for material samples; produce many of the material samples; support the conceptual design of the new RDE injector; manufacture the RDE injector prototypes for testing; and support RDE injector testing, including data capture and post-processing. Georgia Institute of Technology will provide the material model development and application to the design of the RDE injector; review the DofE for completeness; process material samples to extract physical and microstructure qualities; advance the process parameter to microstructure linkage; develop the microstructure-to-fatigue resistance linkage; and support the injector design analysis with process parameter optimization.

The development, implementation, and validation of tools for predicting and verifying microstructural properties, strength, residual stress, and dimensional build characteristics has extremely high relevance for high-temperature high-strength applications that may benefit from additively manufactured parts. Development of a digital twin model of an RDE injector manufacturing process, and an injector that performs in an RDE combustor with a significant reduction in flow loss, will allow the RDE injector to transition to the industrial application of fossil-based power generation.



Modeling of additively manufactured parts leading to low-loss additively manufactured RDE injector.

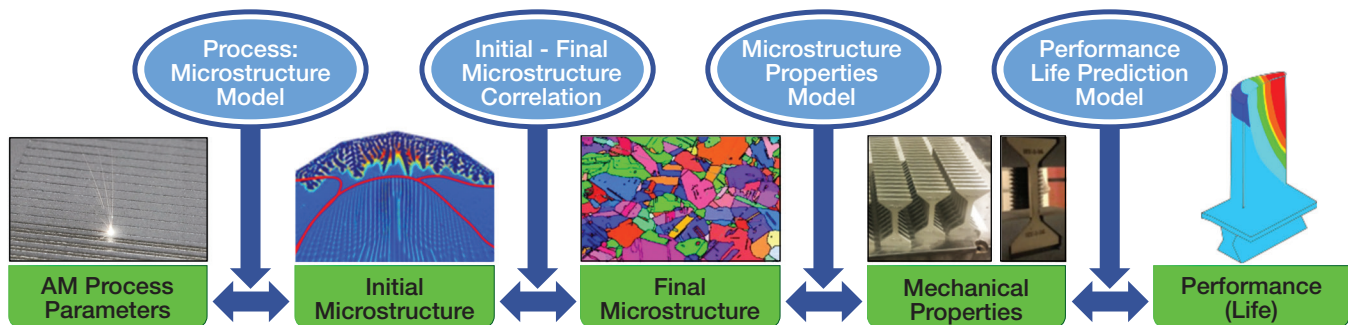
## Computation Tools for Additive Manufacture of Tailored Microstructure and Properties

<b>Performer</b>	Raytheon Technologies Research Center
<b>Award Number</b>	FE0031642
<b>Project Duration</b>	09/01/2018 – 03/31/2021
<b>Total Project Value</b>	\$ 950,244
<b>Technology Area</b>	Coal Utilization Science

United Technologies Research Center will demonstrate the application of computational methods and tools on microstructure evolution and mechanical properties prediction for additively manufactured (AM) nickel-based superalloy parts. Models will be developed in three areas: AM process parameters/microstructure correlation models; correlation between initial microstructure and final microstructure after heat treatment; and final microstructure-to-mechanical-properties relationship. The ability to tailor spatially varying mechanical properties in part by appropriately controlling the microstructure evolution during the AM process will be demonstrated using these models. An integrated computational materials engineering framework that connects process, structure, properties, and performance will be developed and demonstrated.

This project extends computational phase-field models for microstructure evolution—as a function of material processing parameters and crystal plasticity models—fully coupling microstructure, mechanical properties, and service life required for turbine engines.

The tools developed in this project will enable refurbishment of legacy F-Class industrial gas turbines with polycrystalline alloy components built additively by laser powder-bed fusion. These toolsets can be extended to future directionally solidified and single-crystal superalloys produced using AM technology. The time saved by applying validated predictive tools will allow exploration of novel concepts such as tailored property placement based on varying operational requirements within a single part, further unlocking the potential of AM hardware.



An ICME (Integrated Computational Materials Engineering) framework being developed by Raytheon Technologies Research Center that connects Process – Structure – Properties – Performance by four models.

## Large-Scale, Graphics Processing Unit (GPU)-Enhanced Density Functional Tight Binding (DFTB) Approaches for Probing Multi-Component Alloys

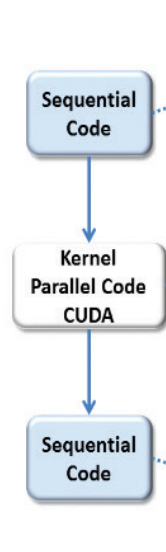
<b>Performer</b>	University of California - Riverside
<b>Award Number</b>	FE0030582
<b>Project Duration</b>	08/01/2017 – 06/30/2021
<b>Total Project Value</b>	\$ 250,000
<b>Technology Area</b>	Coal Utilization Science

The objectives of this project are to develop, analyze, and introduce (1) accurate intermolecular potentials and (2) graphics processing unit enhancements to the density functional tight binding approach for high-throughput ab initio molecular dynamics calculations of multi-component alloys at elevated temperatures. Specifically, this transformative approach utilizes two complementary pathways that will employ a high degree of coordination and communication

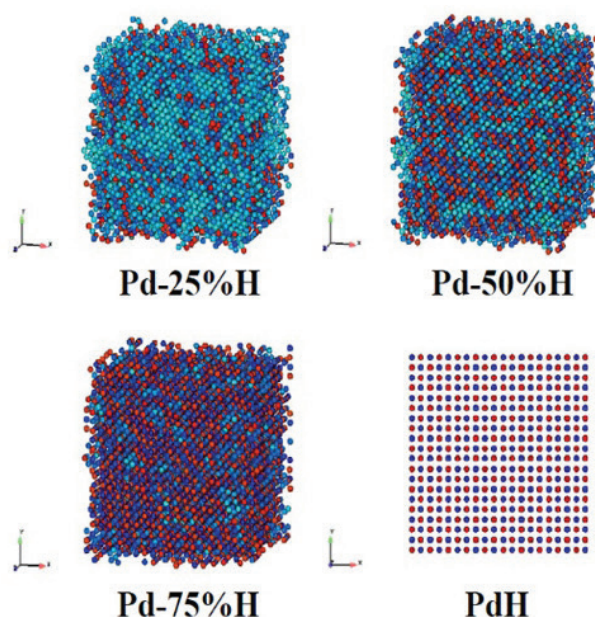
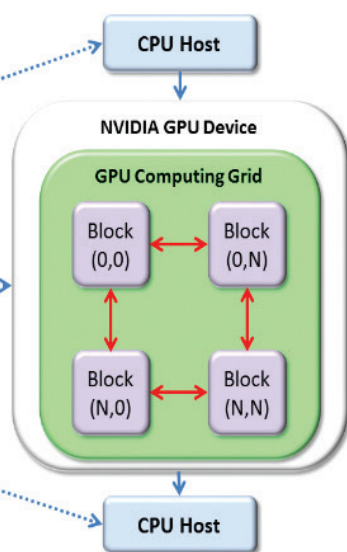
between them to realize a final rigorously sound and validated computational capability upon completion.

The capabilities developed in this project will provide accurate, efficient, and reduced-cost assessment of alloy structural performance at elevated temperature and pressure operational conditions in advanced fossil energy power plants.

### Software Structure



### Hardware Structure



Large-scale simulations of alloy systems.



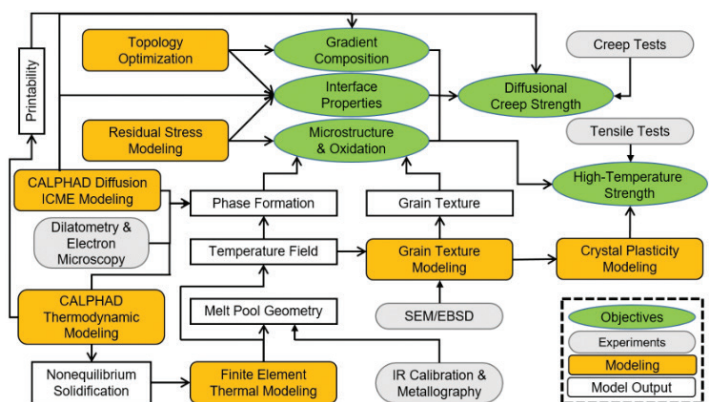
# Integrated Computational Materials and Mechanical Modeling for Additive Manufacturing of Alloys with Graded Structure used in Fossil Fuel Power Plants

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

University of Pittsburgh (Pitt) researchers will develop 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 will be responsible for model development and simulation. United Technologies Research Center (UTRC) will perform 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 will work 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, 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.**

## ABBREVIATIONS

°C.....	degrees Celsius	FSW/P .....	friction stir welding and processing
°F .....	degrees Fahrenheit	FWP .....	Field Work Proposal
ACT.....	accelerated creep testing	GB .....	grain boundary
Al .....	aluminum	GPR.....	Gaussian process regression
AM .....	additive manufacturing	GPU .....	graphics processing unit
AM-GCTJ.....	additively manufactured graded composite transition joint	H282 .....	Haynes 282
ASME .....	American Society of Mechanical Engineers	H <sub>2</sub> O .....	water
AUSC.....	advanced ultrasupercritical	HBCU.....	Historically Black Colleges and Universities
CALPHAD.....	calculation of phase diagrams (methodology)	HIP .....	hot isostatic processing
CFD .....	computational fluid dynamics	HP .....	high-pressure
Co .....	cobalt	HPM.....	High Performance Materials
CO <sub>2</sub> .....	carbon dioxide	HX.....	Hastelloy X
Cr .....	chromium	ICME....	integrated computational materials engineering
CSEF .....	creep strength enhanced ferritic	ICWE .....	integrated computational welding engineering
Cu .....	copper	IN .....	Inconel
DARPA–AIM .....	Defense Advanced Research Projects Agency–Accelerated Insertion of Materials	IN740H.....	Inconel 740H
DFT.....	density functional theory	INL .....	Idaho National Laboratory
DFTB .....	density functional tight binding	LP .....	laser processing
DMW .....	dissimilar metal weldments	MHD .....	magnetohydrodynamic
DNV .....	Det Norske Veritas	Mn.....	manganese
DOE .....	Department of Energy	MOOSE .....	Multiphysics Object-Oriented Simulation Environment
DofE.....	design of experiments	MPa .....	megapascals
DMW .....	dissimilar metal weldment	MWe .....	megawatts electric
DTMM .....	digital twin material model	NETL .....	National Energy Technology Laboratory
EEM.....	extreme environment material	Ni .....	nickel
FCC .....	face-centered cubic	NNS .....	near net shape
FECM.....	Office of Fossil Energy and Carbon Management	O <sub>2</sub> .....	oxygen (molecular)
Fe .....	iron	ODS .....	oxide dispersion strengthened
		OMI.....	Other Minority-Serving Institutions

## ABBREVIATIONS

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  
 R&D ..... research and development  
 RDE ..... rotating detonation engine  
 SAFT ..... synthetic aperture focusing technique  
 sCO<sub>2</sub> ..... supercritical carbon dioxide  
 SE&A ..... systems engineering and analysis

SwRI ..... Southwest Research Institute  
 TCP..... topologically closely packed  
 TTU.....Texas Technological University  
 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:

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<https://energy.gov/fe/plant-optimization-technologies>

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