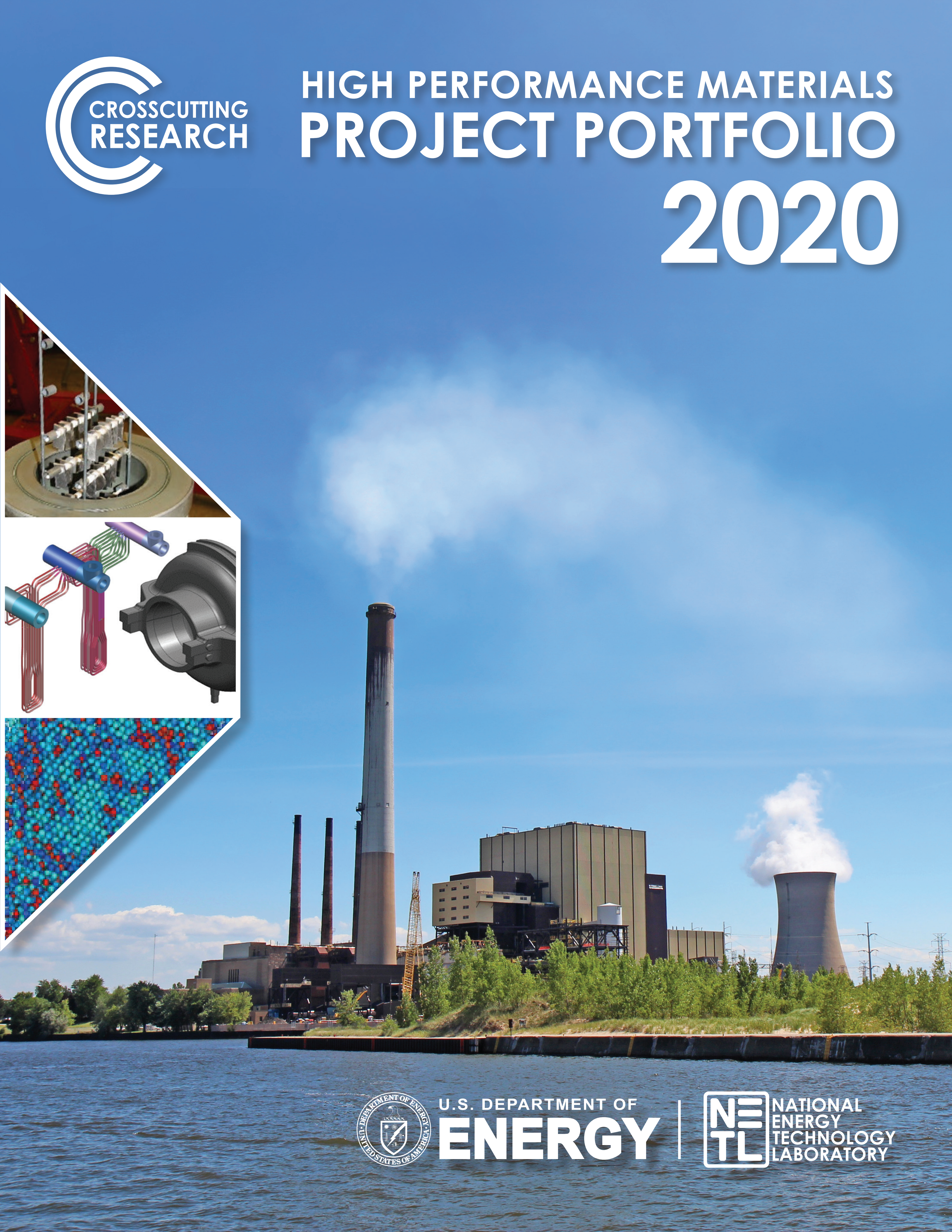
CROSSCUTTING RESEARCH

HIGH PERFORMANCE MATERIALS PROJECT PORTFOLIO 2020



U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

DISCLAIMER

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INTRODUCTION

NETL's Crosscutting Research Program matures novel technologies for commercialization that can enhance new and existing fossil-fired power plants. Six research and development (R&D) programs target enhanced fossil energy systems: High Performance Materials; Sensors, Controls, and Cybersecurity; Modeling, Simulation and Analysis; Water Management; Energy Storage; and University Training and Research.

The goals are to create transformational technologies that improve plant efficiency and security, reduce water consumption, and reduce costs, all under a single research umbrella. The research is leading to enhancements to the fleet such as improved plant efficiency, 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 Program's portfolio, its technologies often have applicability to other energy sectors such as oil and natural gas infrastructure and aviation (both commercial and military).

On behalf of the U.S. Department of Energy's Office of Fossil Energy, NETL pursues crosscutting R&D by collaborating with other government agencies, world-renowned national labs, entrepreneurs, industry, and academic institutions. 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 fossil energy infrastructure, and enable the adoption of cutting-edge data technologies for plant owners and operators.

Sensors and Controls: The Sensors and Controls 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 coal-fired power plants, capable of real-time measurements, improve overall plant efficiencies, and allow for more effective ramp rates. Given the crosscutting nature of sensors and controls, these technologies will also benefit natural gas power generation and other harsh-environment applications.

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

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

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, and Computational Materials Design.

Modeling, Simulation and Analysis: Modeling, Simulation and Analysis (MSA) 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 MSA 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 analyses that are essential in informing and deciding between priority technology choices. 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: FE's Advanced Energy Storage program aims to address the needs and challenges of fossil assets through the integration of energy storage technologies. As the penetration of variable renewable energy increases, energy storage at the generation site will be essential to a resilient and flexible electricity network. Energy storage also benefits the environment through optimization of fossil generation and by enabling additional renewables on the grid to reliably transmit their energy to end users. Program activities include plant- and system-level analyses, conceptual and detailed engineering designs, breakthrough R&D on innovative energy storage concepts, and targeted R&D on component and system-integrated energy storage technologies.

University Training and Research: University Training and Research supports two of the longest-running university training programs, the Historically Black Colleges and Universities (HBCU) and Other Minority Institutions (OMI) and the University Coal Research (UCR) programs, to support the education of students in the area of coal science is promoted through grants to U.S. colleges and universities that emphasize FE 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. The Outreach Initiative provides opportunities for qualified students and post-doctoral researchers to hone their research skills with NETL's in-house scientists.

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:

- Enhance the Nation's high-temperature materials supply chain.
- Develop high-throughput advanced manufacturing processes for fossil applications. These applications typically feature materials capable of withstanding extreme environments and require the fabrication of components that are larger than for aviation engines (where additive manufacturing is more well established).
- 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 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 41 high-performance materials projects within the Crosscutting High Performance Materials Program. Each of the pages reporting on projects describes the technology, status, accomplishments, project goals, and overall benefits.

ADVANCED MANUFACTURING

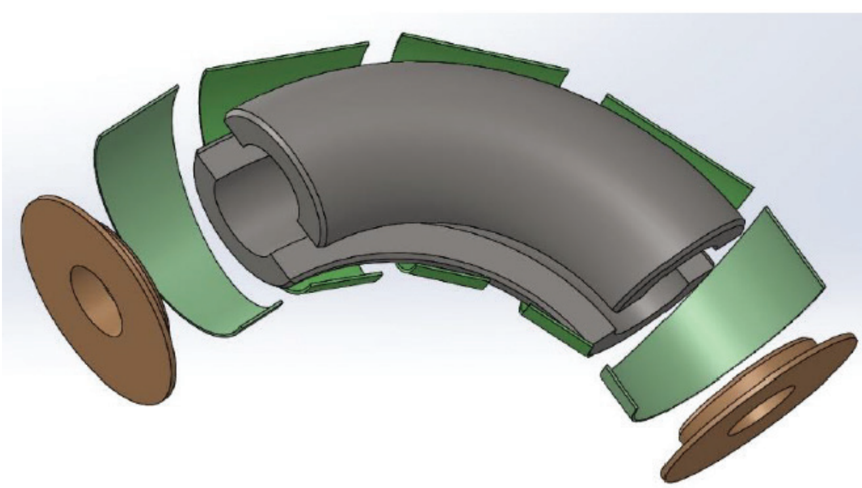
Low-Cost HIP Fabrication of Advanced Power Cycle Components and PM/Wrought IN740H Weld Development

Performer	**General Electric (GE) Company**
Award Number	FE0031818
Project Duration	10/01/2019 – 03/31/2021
Total Project Value	$ 1,299,505
Collaborators	Electric Power Research Institute, Inc.; Special Metals; Wyman-Gordon
Technology Area	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_2) 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.



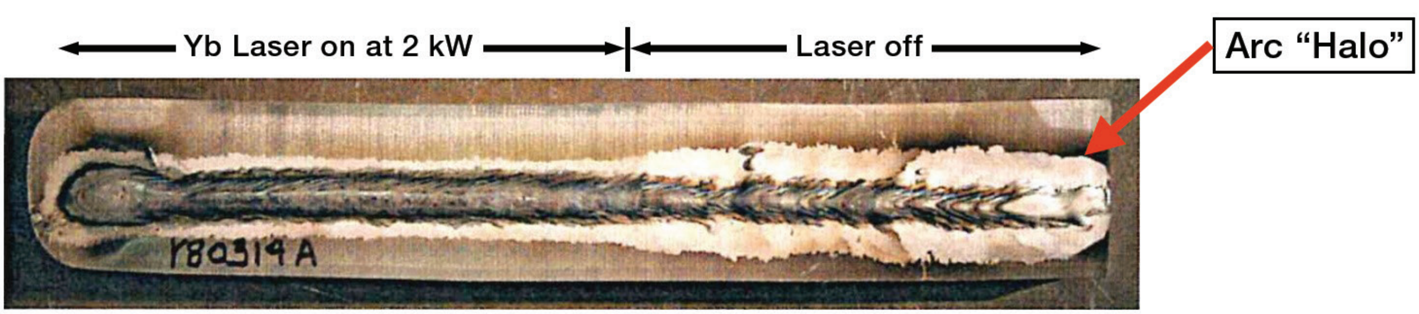
Virtual assembling of the HIP tooling for the IN740H pipe elbow.

Multi-pass Hybrid Laser Arc Welding of Alloy 740H

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

Idaho National Laboratory will employ hybrid laser arc welding techniques to initially weld thick weld groove land areas (approximately 0.5 inches 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.



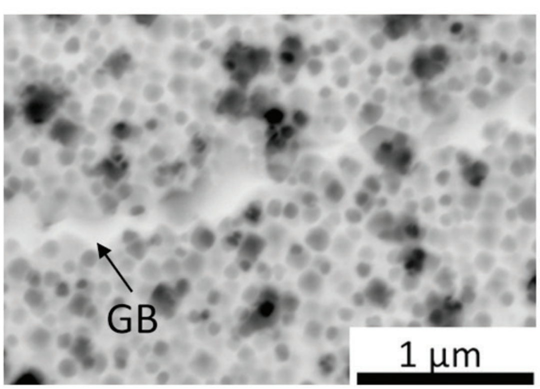
The benefits of laser stabilization in hybrid laser arc welding on Inconel 740H.

Additive Manufacturing of High Gamma Prime Alloys

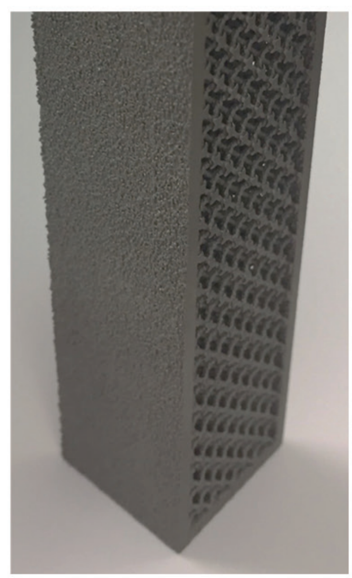
Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA127
Project Duration	09/01/2017 – 03/31/2020
Total Project Value	$ 424,000
Collaborator	Siemens
Technology Area	Plant Optimization Technologies

NETL is partnering with Oak Ridge National Laboratory (ORNL) to develop advanced components from high gamma prime alloys (Haynes 282/Nimonic 105) via innovative manufacturing approaches to enable high temperature/high pressure operation and realize high plant cycle efficiency for advanced ultrasupercritical (AUSC) steam systems (with relevance to gas turbines). Several key challenges currently confront the additive manufacturing (AM) processes for high gamma prime alloys. It is universally recognized that the internal microstructures and performance under load are dependent on the manufacturing process. Due to the large parameter sets applicable in AM processes and their impact on achievable materials properties and quality, a design-of-experiments approach will be utilized to achieve the optimal crack-free microstructure with acceptable density.

For AM of high gamma prime alloys, where the understanding of the effects of feedstock properties, deposition rates, thermal history, cooling rates, defect formation, and residual stress are still in an early phase, the design-of-experiments approach will achieve the optimal part properties (density/mechanical properties), surface finish and performance, similar to the rolled plate material. Collaboration between ORNL and Siemens will provide the unique opportunity of developing the process parameters, part microstructure/surface finish, and bulk properties for Haynes 282 and Nimonic 105. The final goal is to fabricate Haynes 282 and Nimonic 105 components that are of interest to the AUSC program.



Back scattered scanning electron images of alloy 282 fabricated by electron beam melting showing the grain boundary (GB) carbides and fine gamma prime precipitates in the as-built condition.



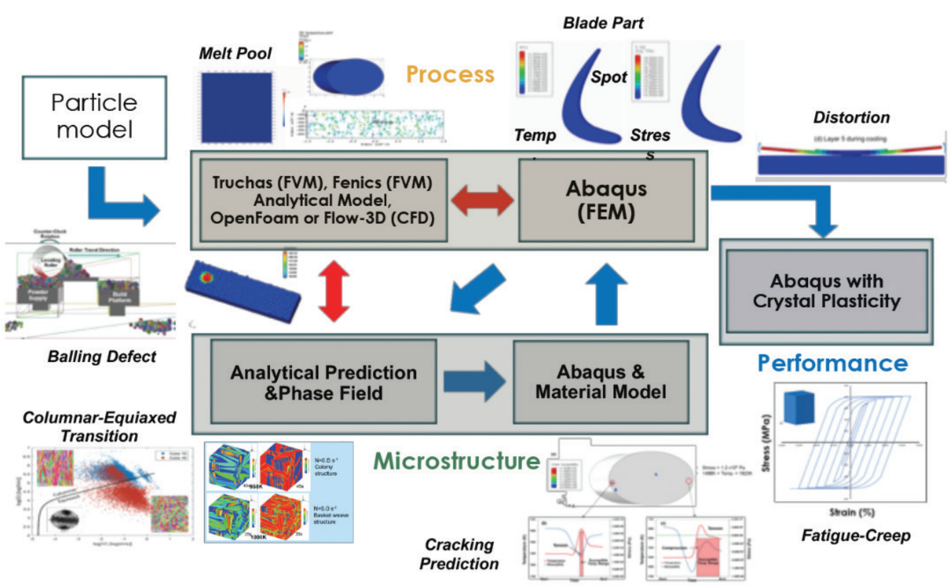
Example of a complex Haynes 282 mesh structure fabricated by electron beam melting.

Components Fabricated by Additive Manufacturing

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA128
Project Duration	10/01/2018 – 09/30/2021
Total Project Value	$ 900,000
Collaborator	Siemens
Technology Area	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.

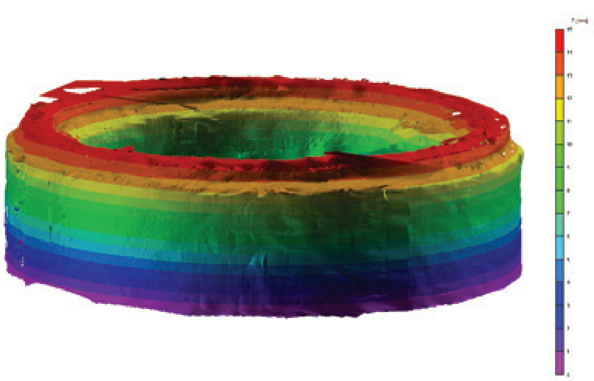
Development of Functionally Graded Transition Joints to Enable Dissimilar Metal Welds

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA151
Project Duration	07/01/2019 – 09/30/2020
Total Project Value	$ 1,000,000
Technology Area	Plant Optimization Technologies

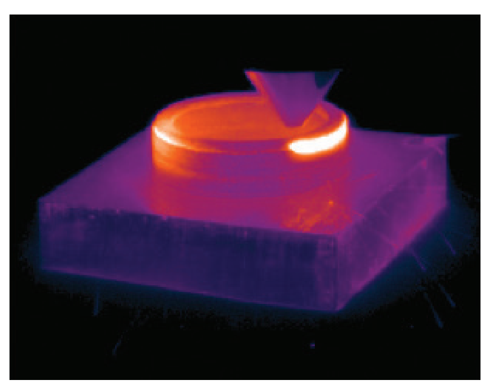
Oak Ridge National Laboratory will weld dissimilar metals using functionally graded transition joints that exhibit high resistance to creep and fatigue and high microstructural stability. The primary focus of the project will be on joining ferritic steels to austenitic steels, in particular alloys that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



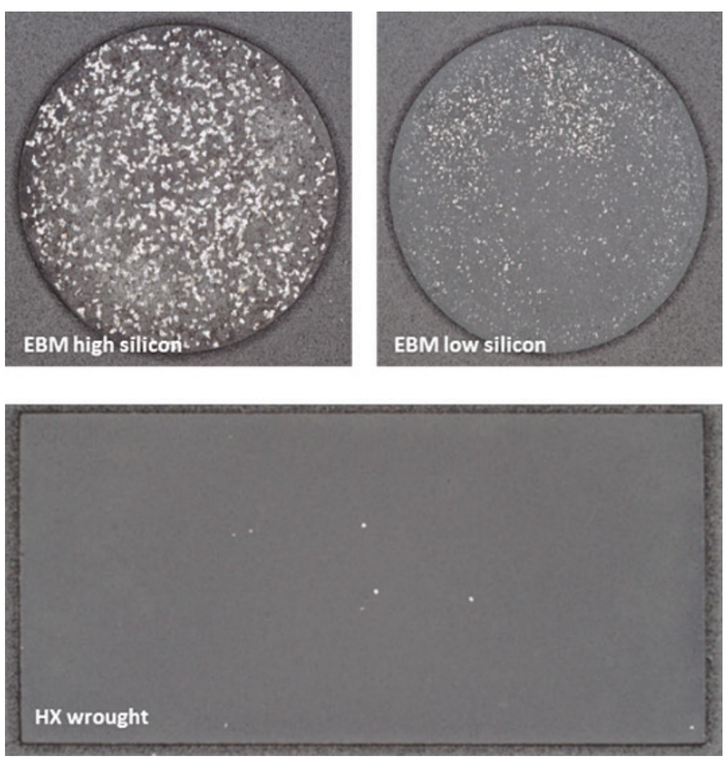
IR image showing temperature distribution with build height.

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

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA119
Project Duration	09/01/2015 – 06/30/2020
Total Project Value	$ 954,000
Technology Area	Plant Optimization Technologies

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

The technology will be used to produce high-temperature gas turbine components as well as similar-sized components for other advanced fossil energy applications.

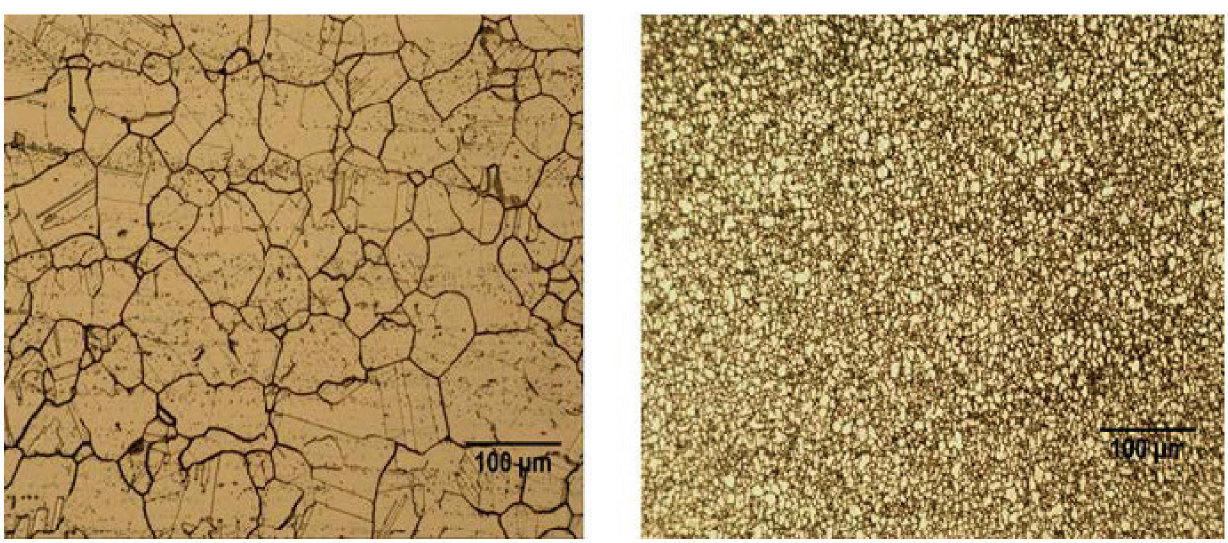


No spallation for wrought HX 4x 100 hours at 950 °C.

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

Performer	**Pacific Northwest National Laboratory (PNNL)**
Award Number	FWP-71843
Project Duration	10/01/2018 – 09/30/2021
Total Project Value	$ 1,120,000
Technology Area	Plant Optimization Technologies

The goal of this project is to determine the advantages of laser and friction stir processes when applied to the processing of nickel-based alloys used in extreme operating environments found in fossil energy power systems. This project will investigate and demonstrate an integrated approach using both laser processing (LP) and friction stir welding and processing (FSW/P) to join, repair, and return to service nickel alloy castings and wrought fabrications such as hot gas path components in gas turbine applications. The 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, AUSC and sCO_2 heat exchangers).



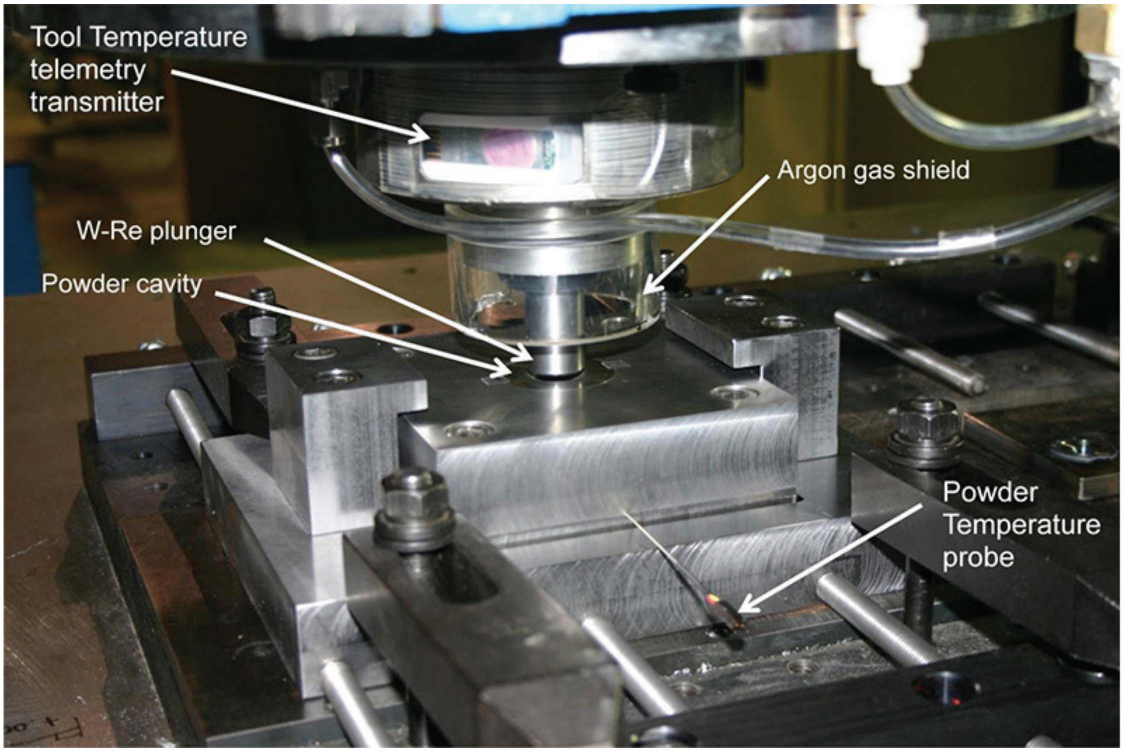
Microstructure comparison of Haynes 282 base material (left) and FSW weld nugget (right).

Low Cost Fabrication of ODS Materials

Performer	**Pacific Northwest National Laboratory (PNNL)**
Award Number	FWP-60098
Project Duration	10/01/2010 – 09/30/2020
Total Project Value	$ 735,000
Technology Area	Plant Optimization Technologies

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

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



Friction extrusion die at Pacific Northwest National Laboratory.

Solid State Joining of Creep Enhanced Ferritic Steels

Performer	**Pacific Northwest National Laboratory (PNNL)**
Award Number	FWP-66059
Project Duration	10/01/2014 – 09/30/2020
Total Project Value	$ 1,075,000
Technology Area	Plant Optimization Technologies

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

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

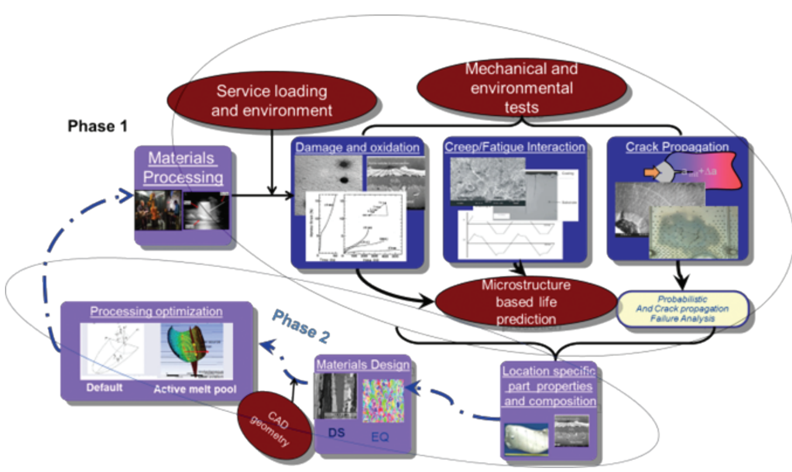
Flat plate friction stir welds in HSLA65 plate.

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

Performer	**United Technologies Research Center (UTRC)**
Award Number	FE0031821
Project Duration	10/01/2019 – 03/31/2021
Total Project Value	$ 1,249,916
Collaborator	Siemens
Technology Area	Plant Optimization Technologies

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

The project will augment the WAAM process to produce fossil energy system components with tailored properties though functionally graded microstructure. In phase 1, a physics-driven process model will be used to generate a novel build strategy that can produce directionally solidified and equiaxed morphology in the same component while utilizing localized heating, cooling, and modified feedstocks. 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.

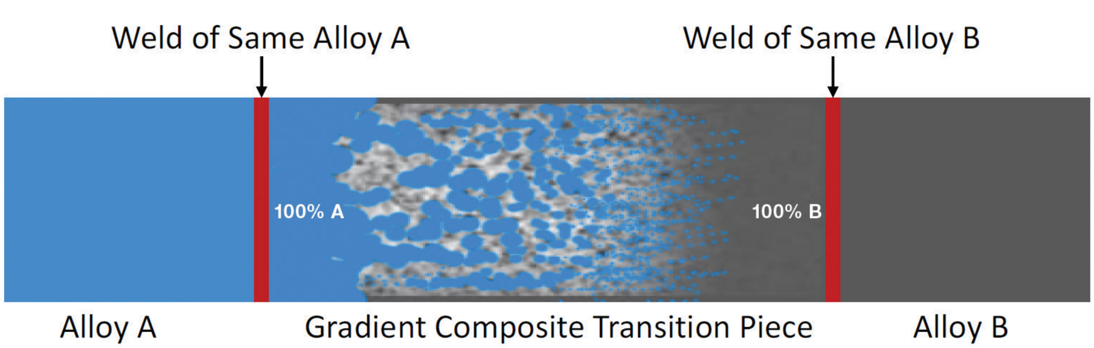
Additively Manufactured Graded Composite Transition Joints for Dissimilar Metal Weldments in Utra-Supercritical Power Plant

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	
Technology Area	Plant Optimization Technologies	

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

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

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



Concept of additively manufactured graded transition joint.

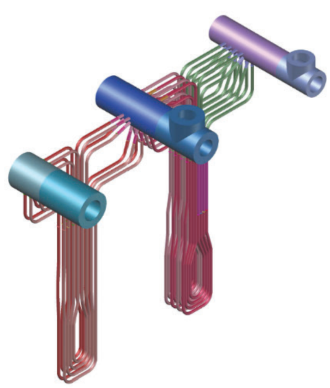
ADVANCED STRUCTURAL MATERIALS

Advanced Ultra-Supercritical Component Testing

Performer	**Energy Industries of Ohio, Inc.**
Award Number	FE0025064
Project Duration	11/01/2015 – 09/30/2021
Total Project Value	$ 26,750,822
Collaborators	AECOM; Alstom Power, Inc.; Electric Power Research Institute, Inc.; GE Power and Water; MetalTek International; Riley Power; Special Metals; Thermal Engineering; Youngstown Thermal
Technology Area	Plant Optimization Technologies

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

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



AUSC superheater/reheater assembly.

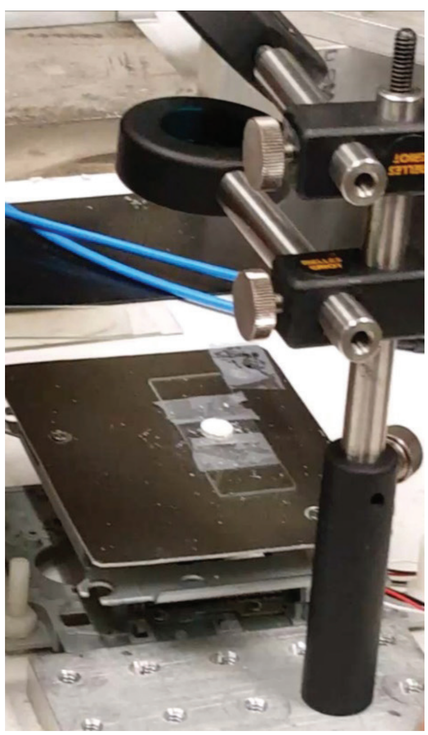
Nozzle carrier casting.

Novel High Temperature Carbide and Boride Ceramics for Direct Power Extraction Electrode Applications

Performer	**Florida International University**
Award Number	FE0026325
Project Duration	10/01/2015 – 09/30/2020
Total Project Value	$ 249,970
Technology Area	University Training and Research

NETL is partnering with Florida International University to develop nano-carbide and -boride ceramic solid solution and related composites via novel synthesis and processing and to understand the fundamental composition-processing-structure-property relationships for materials such as potential hot electrodes for magnetohydrodynamic (MHD) direct power extraction systems. Basic research on new high-temperature ceramic materials, including novel means of synthesis and processing, will be performed. Fundamental knowledge will be developed and leveraged to design direct power extraction applications for cleaner and more efficient power generation using fossil fuels.

This research will provide insights into how fundamental composition-processing-structure-property relationships will support development of these materials for a broad range of applications from energy to aerospace. This research could also significantly impact the development of high-temperature MHD electrodes as well as the fields of advanced ceramics and high-temperature materials science and could lead to dramatic reductions in the time and energy required during the materials sintering process, resulting in less costly high-temperature ceramic materials.



Green body formation via laser cutting.

Advanced Alloy Development

Performer	National Energy Technology Laboratory (NETL)
Award Number	FWP-1022406
Project Duration	04/01/2018 – 03/31/2021
Total Project Value	$ 10,718,127
Technology Area	Plant Optimization Technologies

NETL's Research and Innovation Center's Advanced Alloy Development Field Work Proposal (FWP) is focused on developing high-performance materials to improve efficiencies in the existing fleet and enable next generation 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 & Market Analysis. Techno-economic and market analysis to provide alloy production, supply chain issues, and performance/cost benefits of high-performance materials on fossil fuel power generation plants [e.g., advanced ultra-supercritical (AUSC) Rankine cycles] enabled by advanced alloys.

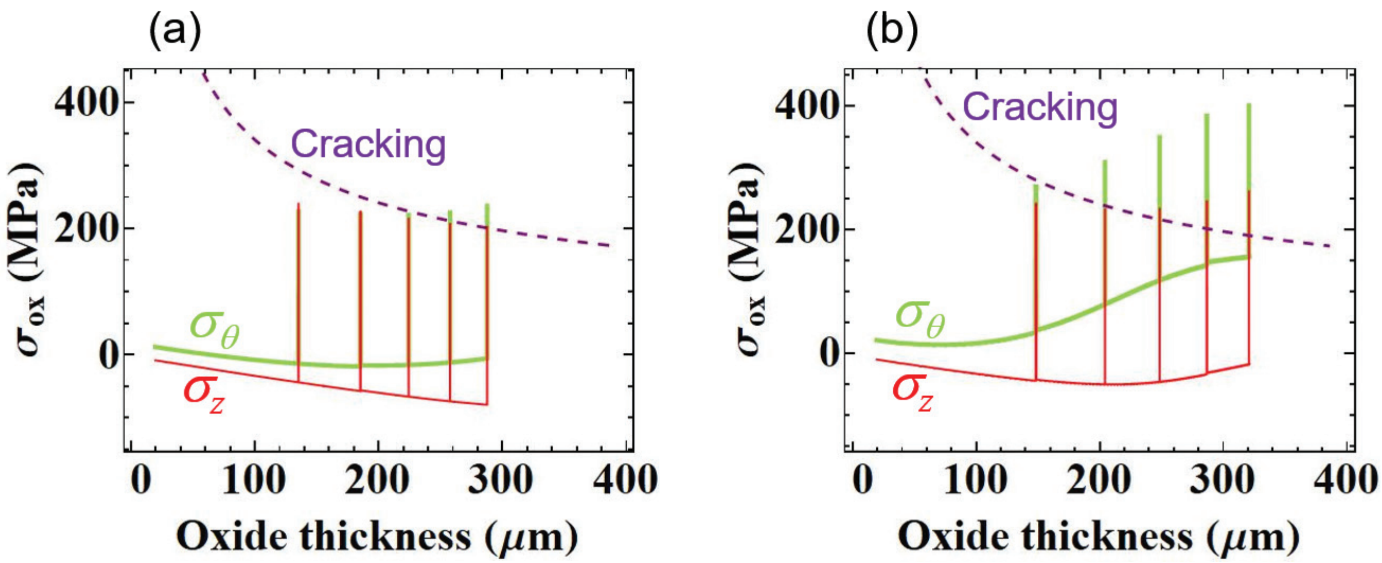
Computational Design and Simulation—Use computational materials modes, multi-scale characterization simulations of microstructural features, and cutting-edge data analytics to guide and accelerate alloy design and manufacturing development and improve component service life prediction.

Processes, Manufacturing, and Properties— Increase temperature capabilities of steels and nickel alloys to lower the cost advance FE systems (AUSC and sCO_2) and improve the existing fleet. Develop and demonstrate at pilot industrial scales improved manufacturing processes to produce advanced alloys with improved service life performance.

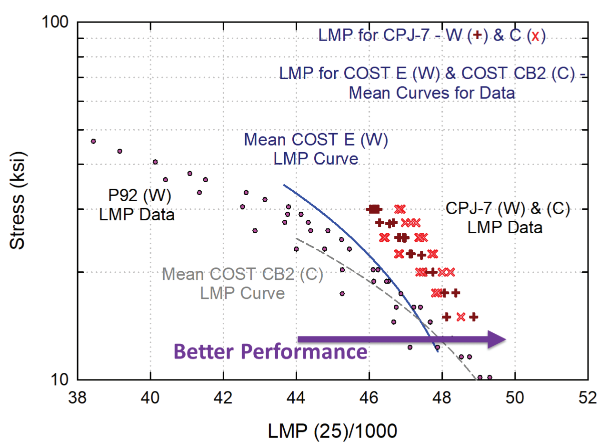
Materials for sCO_2 Power Cycles: Alloy Performance—Determine whether available AUSC power plant materials are suitable for fossil fuel supercritical carbon dioxide (sCO_2) service in terms of temperature and stress, and if they are, assess the potential physical and mechanical consequences of their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

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

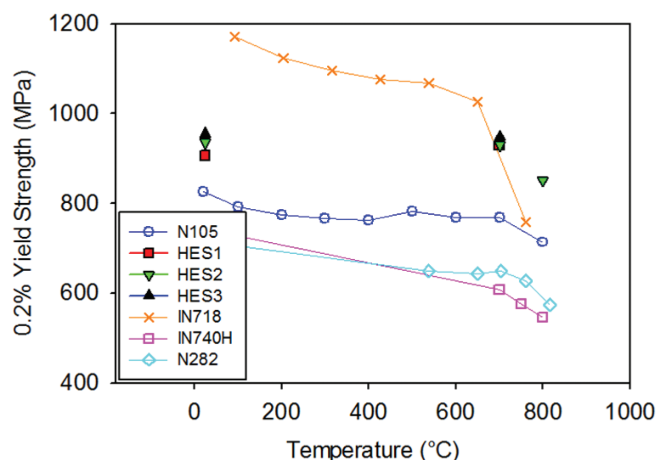
The structural materials and manufacturing processes researched in this FWP are needed to lower the cost and improve the performance of fossil-based power-generation. Additionally, the development and utilization of computational simulation and broad-based data analytic tools can further reduce the time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



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 streels, 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).

Creep-Fatigue-Oxidation Interactions: Predicting Alloy Lifetimes under Fossil Energy Service Conditions

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA115
Project Duration	10/01/2013 – 08/31/2020
Total Project Value	$ 1,500,000
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to generate pertinent creep-fatigue data and develop new lifetime models to help accurately predict the lifetimes of fossil fuel power plant components that are subjected to flexible operation (e.g., load cycle following of renewable power generation). Such flexible operation can cause thermal-mechanical fatigue of components over long periods, resulting in their premature failure. Most existing coal-fired power plants were not designed for flexible operation, and new advanced fossil fuel plants may need to include flexible operation in their thermal/mechanical design.

Improvements to creep-fatigue data and lifetime models will advance the development of advanced power plant designs, improve efficiency and operational flexibility, and reduce operating costs.

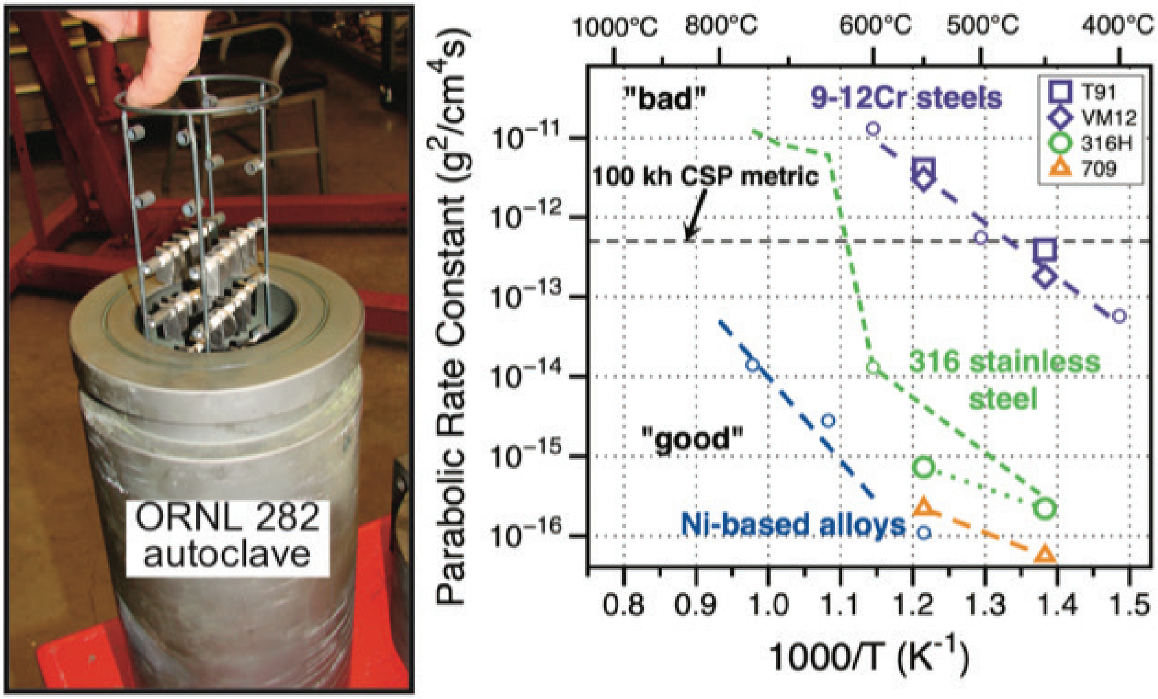
Left: Servo-hydraulic creep-fatigue machine.
Right: Thermal cyclic creep machines allowing testing in steam.

Effect of Impurities on Supercritical Carbon Dioxide Compatibility

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

The proposed work will study the effect of impurities (e.g., O_2; H_2O) on compatibility of structural materials in supercritical carbon dioxide (sCO_2) Brayton cycle systems, particularly for direct-fired systems. High impurity levels (0.25–1 percent) have been found to increase reaction rates of both Fe- and Ni-based alloys at 750 degrees Celsius (°C)/300 bar (30 megapascals; MPa). Further work is needed to isolate O_2 and H_2O 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_2 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_2 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_2 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_2 community and materials suppliers, as well as to the high-temperature materials community in general, as appropriate.

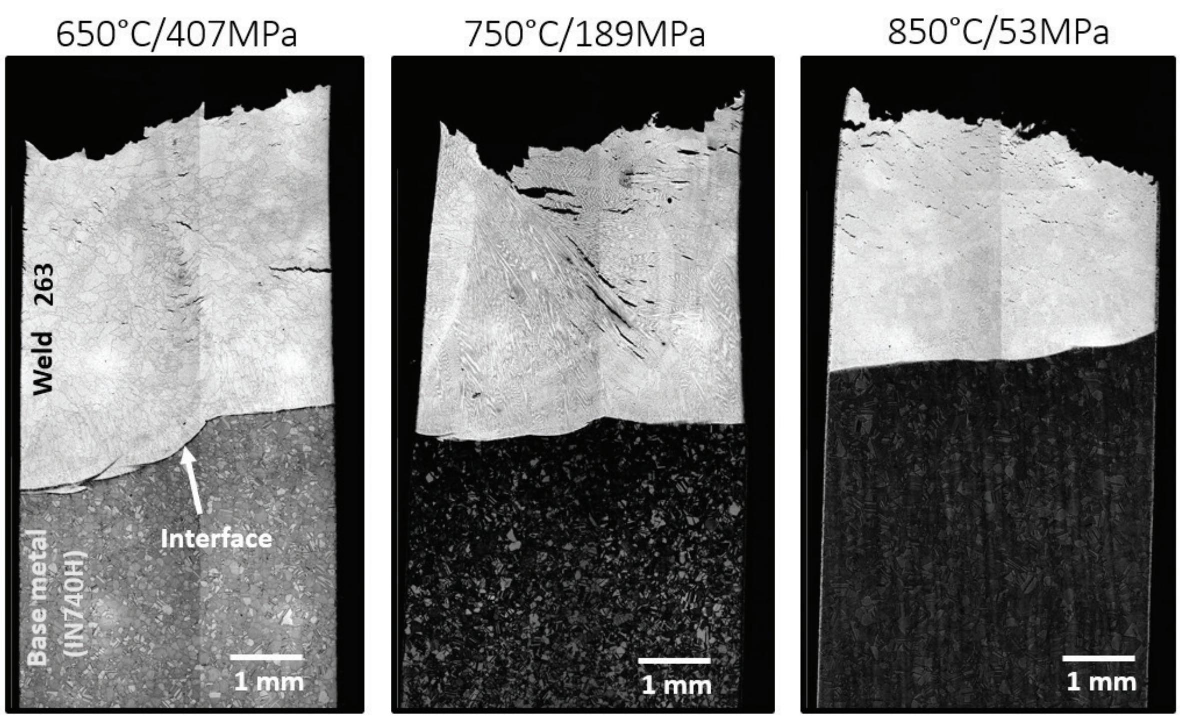


ORNL is evaluating structural steels at 450°–650°C in 30MPa supercritical CO_2 using laboratory autoclaves (left) to determine under what conditions the reaction rates are low enough for power generation applications. On the right, an Arrhenius plot of parabolic rate constants compares rate constants measured on this project to literature values.

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

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

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 degrees Celsius (°C; 1400 °F) and 35 megapascals (MPa; 5000 psig). In particular, this project focuses on evaluating materials from near-to-full-scale components, such as Haynes 282 large rotor forging, half-valve body casting, and steam turbine nozzle carrier casting, to provide 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.



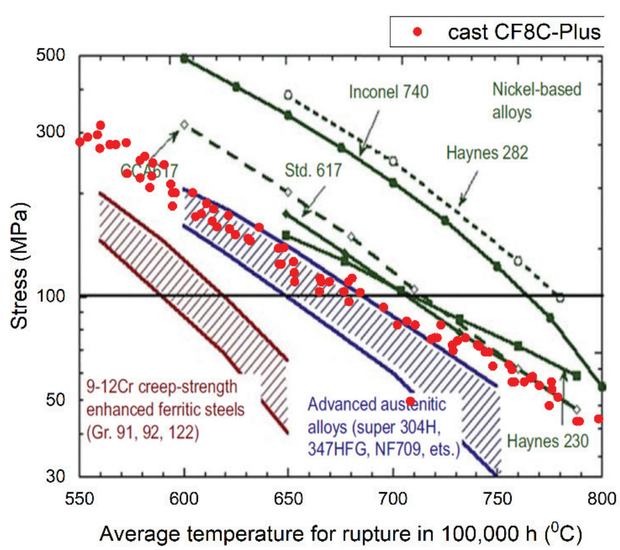
Cross-section view of creep rupture specimens of Inconel 740H cross-weld made with alloy 263 filler metal.

Low Cost High Performance Austenitic Stainless Steels for A-USC

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

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.



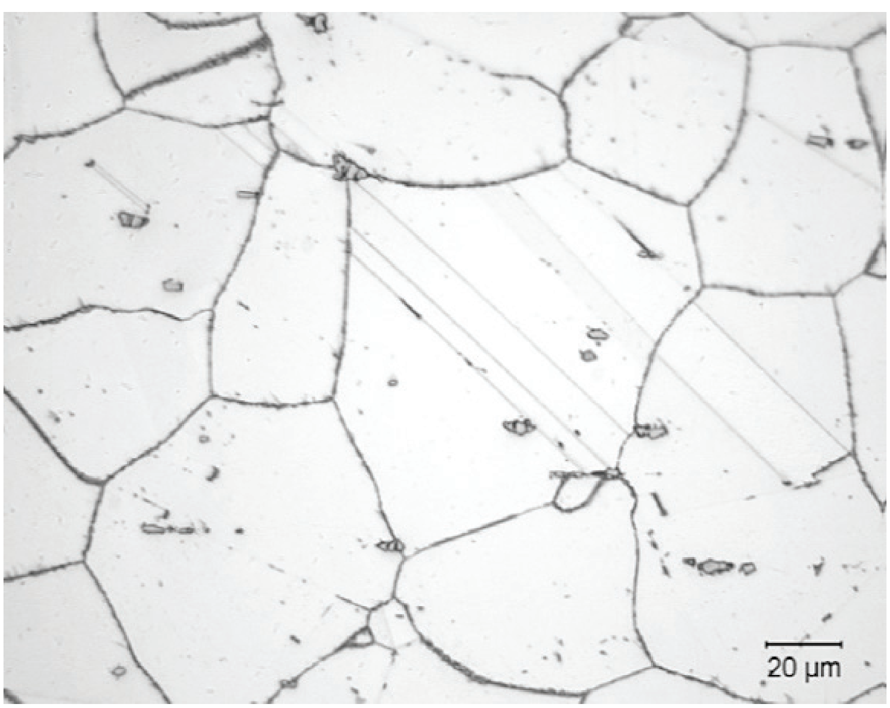
Comparison of 100,000 h creep-rupture strength as a function of temperature between cast CF8C-Plus and other alloy classes.

Materials Qualification and Deployment for High Efficiency Coal Fired Boilers

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA117
Project Duration	04/01/2015 – 03/31/2020
Total Project Value	$ 820,000
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to address materials issues relevant to qualifying and deploying a nickel (Ni)-based alloy for a new application in an advanced ultrasupercritical coal-fired boiler. The project will deploy Haynes 282 (H282) alloy for application in superheaters, reheaters, and steam delivery pipes by completing base metal and cross-weld creep and tensile testing needed for an American Society of Mechanical Engineers (ASME) Boiler and Pressure Vessel Code Case and the associated microstructural analyses needed for assurance of boiler-relevant lifetimes. Lab work will focus on tensile and creep testing of the base metal and cross welds in the 1,100 to 1,700 °F temperature range.

The goal of this project is to generate the laboratory mechanical properties data needed to obtain ASME Code qualification of single aged H282 nickel superalloy for use in pressure-bearing components of coal-fired boilers and other high-temperature power generation equipment. Microstructural characterization will provide insights into failure mechanisms that will help support extrapolation methods of the lab creep test data to estimated creep strength at 100,000 hour life.



H282 microstructure in age hardened condition.

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

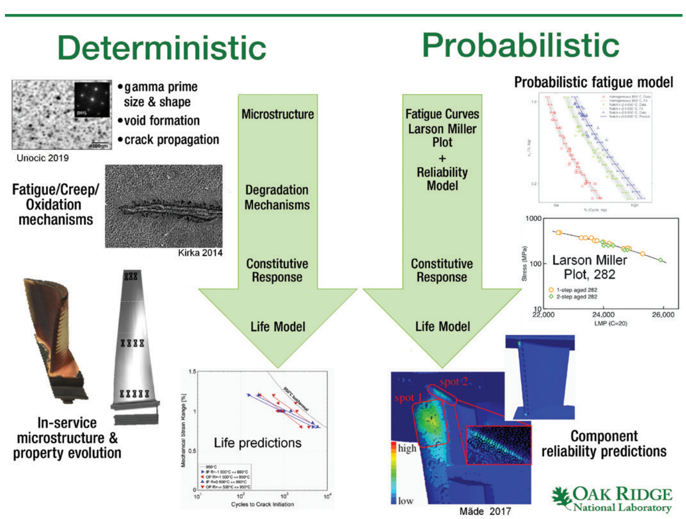
Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA137
Project Duration	10/01/2018 – 09/30/2021
Total Project Value	$ 900,000
Technology Area	Plant Optimization Technologies

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

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

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

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

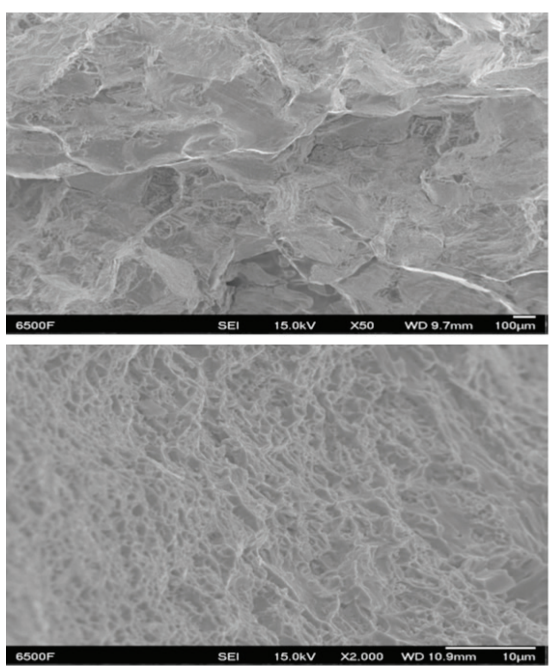


Properties of Advanced Ni-Based Alloys for A-USC Steam Turbines

Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA125
Project Duration	02/01/2016 – 08/31/2020
Total Project Value	$ 2,160,000
Technology Area	Plant Optimization Technologies

NETL is partnering with ORNL to evaluate the behavior of high-temperature materials to complement the efforts of the Advanced Ultrasupercritical (AUSC) Steam Turbine Materials Consortium in qualifying alloys for steam turbine designs required for operation under AUSC steam conditions of 760 degrees Celsius (°C)/1400 degrees Fahrenheit (°F) and 345 bar/5000 psi, and in ensuring that any limitations of current materials are overcome. This project will perform creep testing and microstructural characterization of a large cast valve body of Haynes 282 alloy; evaluate long-term creep resistance of a large forging of Haynes 282 alloy, including the effects of fine grain size; evaluate steam effects and pre-test microcracks on the fatigue behavior of the large forging of Haynes 282 alloy; perform microstructural characterization and longer-term creep testing for dissimilar metal welds of Inconel 740H pipe joined to Haynes 282 alloy valve casting; develop constitutive equations or predictive models and upgrade the damage evaluation and life-prediction criteria; and perform tests to assess the effects of CO_2 on mechanical behavior.

This project will reduce the quantity and cost of components made from nickel superalloys by developing more precise mechanical behavior data that can be used to produce more accurate models of the mechanical behavior of these components under varying high temperatures and applied stress conditions.

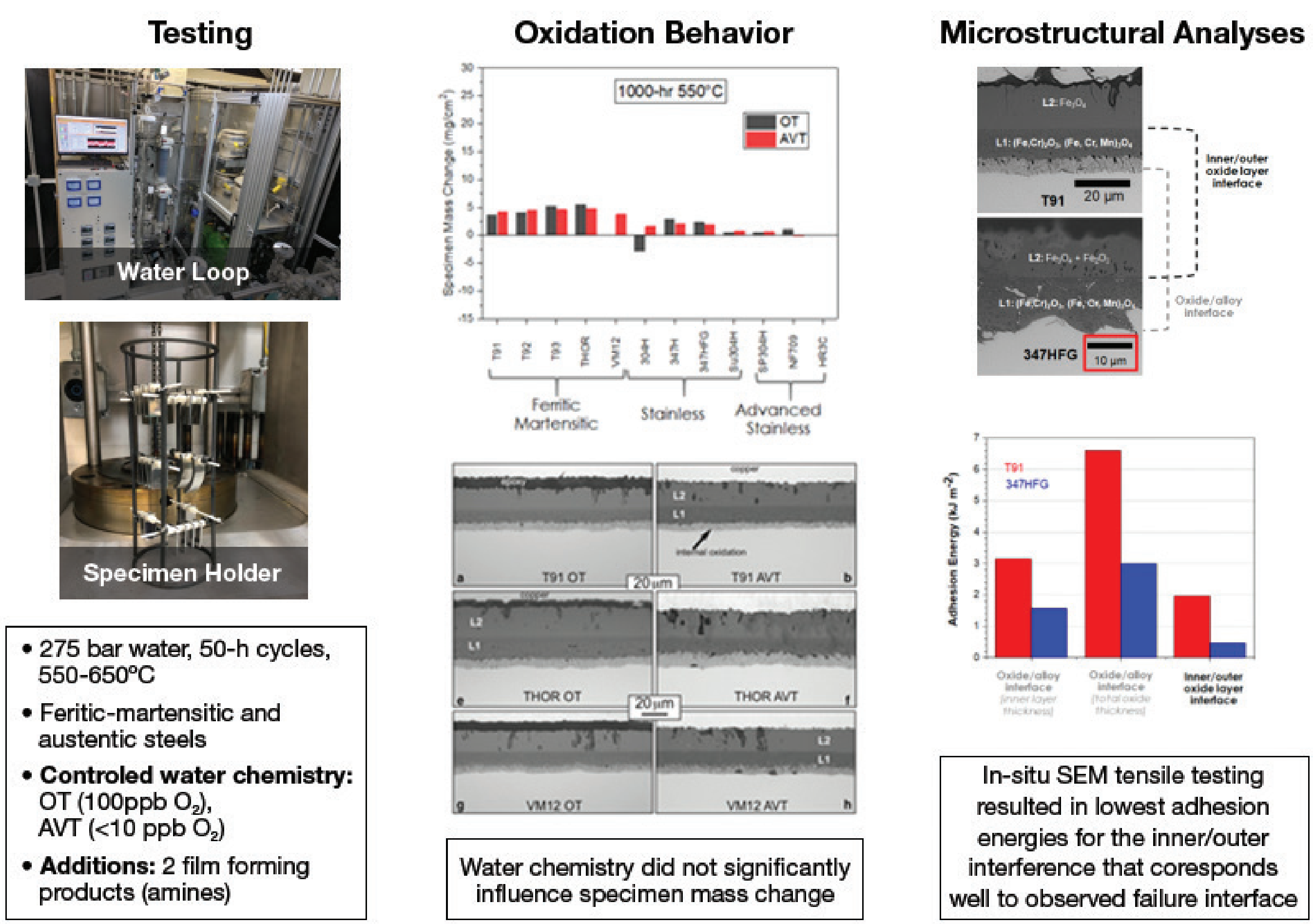


Cast Haynes 282 fractures mainly along heavily precipitated dendrite colony boundaries.

Steamside Oxidation Issues in Current Coal-Fired Boilers

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

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



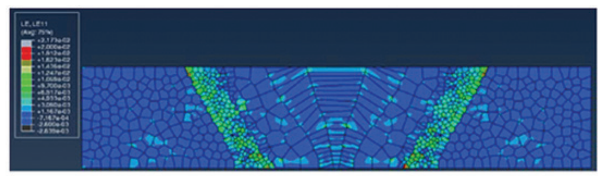
Weldability of Creep Resistant Alloys for Advanced Power Plants

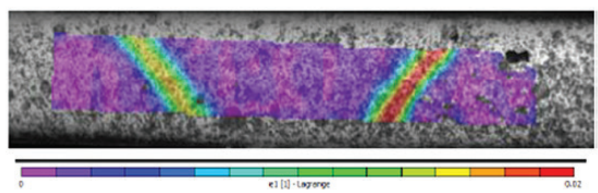
Performer	**Oak Ridge National Laboratory (ORNL)**
Award Number	FWP-FEAA118
Project Duration	10/01/2013 – 06/30/2020
Total Project Value	$ 1,800,000
Technology Area	Plant Optimization Technologies

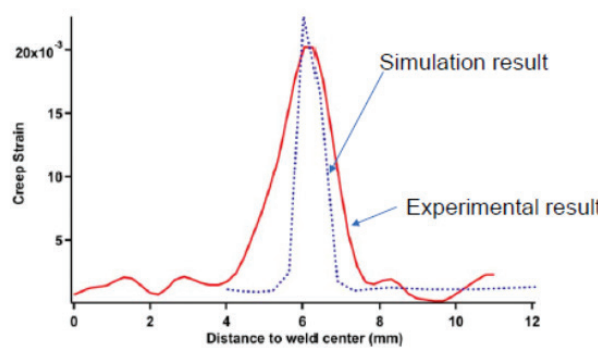
NETL is partnering with ORNL to develop practical engineering solutions to two key issues regarding the weldability of high-temperature creep-resistant alloys used in advanced fossil energy power plants: (1) the reduced creep strength of the weld region versus the base metal, and (2) welding of dissimilar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







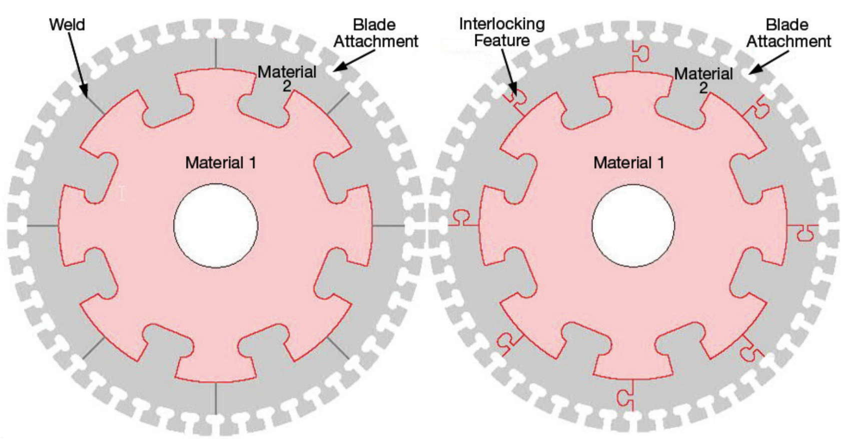
Top: Modeling result.
Middle: Experimental result.
Bottom: Simulation result shows agreement with experiments.

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

Performer	**Siemens Corporation**
Award Number	FE0031824
Project Duration	10/01/2019 – 03/31/2021
Total Project Value	$ 1,408,866
Technology Area	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 degrees Celsius 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

Performer	**Tennessee Technological University**
Award Number	FE0031820
Project Duration	10/01/2019 – 03/31/2021
Total Project Value	$ 1,030,754
Collaborators	Eastern Plating; Oak Ridge National Laboratory; Purdue University; Siemens
Technology Area	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.

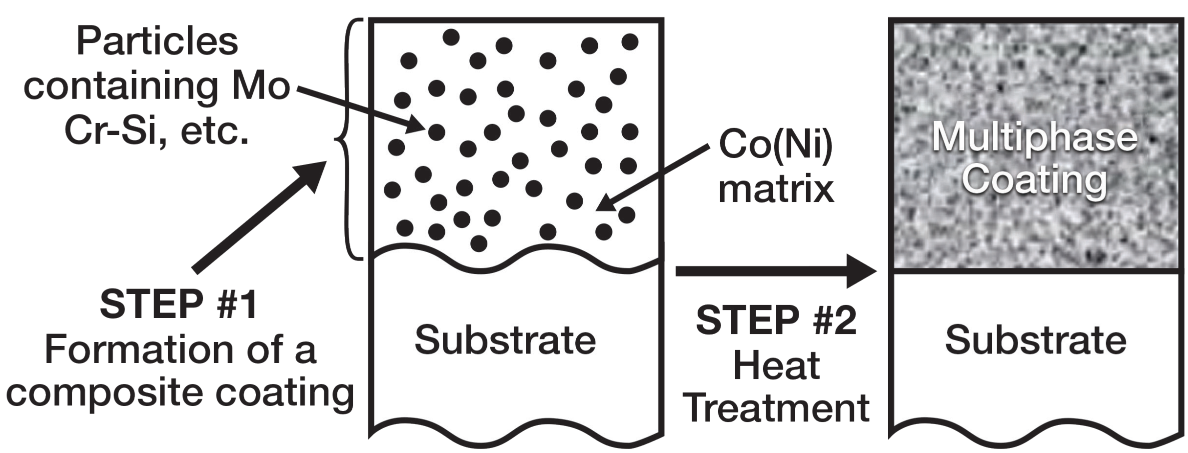


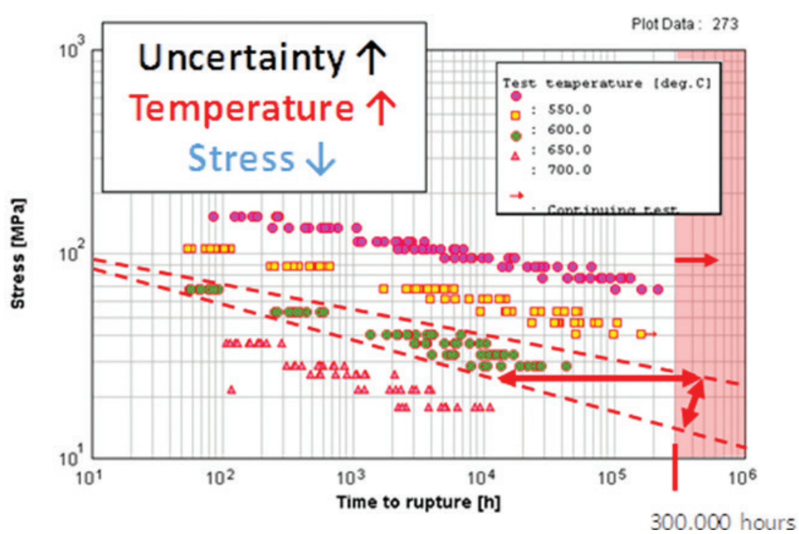
Illustration of the electro-codeposition coating process.

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

Performer	**University of Texas at El Paso**
Award Number	FE0030331
Project Duration	09/01/2017 – 02/28/2021
Total Project Value	$ 400,000
Technology Area	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.



Creep-rupture of 9Cr-1Mo tube.

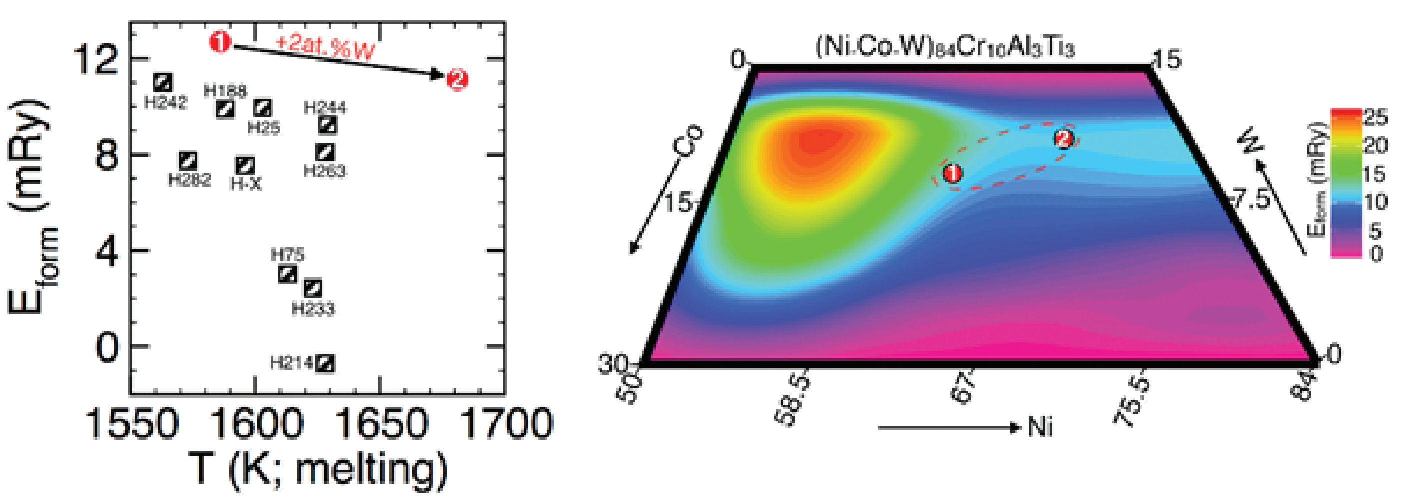
COMPUTATIONAL MATERIALS DESIGN

Predictive Design of Novel Ni-based Alloys

Performer	**Ames National Laboratory**
Award Number	FWP-AL-19-510-097
Project Duration	04/08/2019 – 09/30/2021
Total Project Value	$ 750,000
Technology Area	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 to computational design and optimization of the alloys: (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 Eform varies with experimentally determined Tm for common Haynes alloys. Right graphic shows (on a reduced pseudo-quaternary plot) how Eform varies with content of the refractory element; W, with Ni and Co.

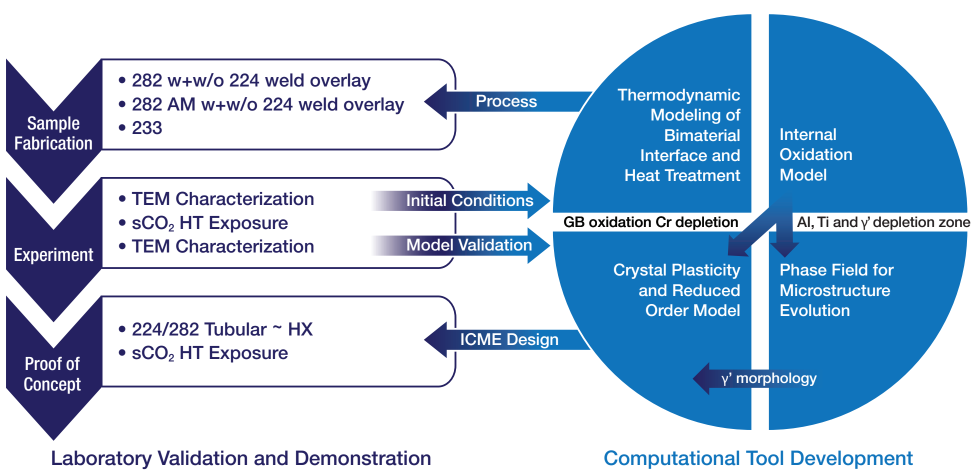
ICME for Advanced Manufacturing of Nickel Superalloy Heat Exchangers with High Temperature Creep Plus Oxidation Resistance for Supercritical CO_2

Performer	Det Norske Veritas (DNV) GL USA, Inc.
Award Number	FE0031631
Project Duration	10/01/2018 – 09/30/2020
Total Project Value	$ 937,500
Collaborator	Ohio State University
Technology Area	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_2 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_2.

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 AM for HT HX Systems



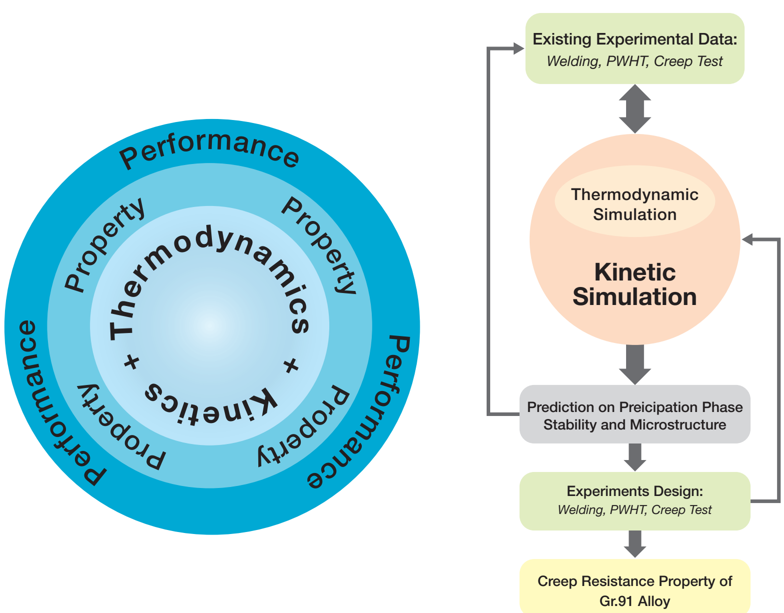
Computational tool development pathway to support multi-material additive manufacturing for high-temperature heat exchange systems.

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

Performer	**Florida International University**
Award Number	FE0027800
Project Duration	08/01/2016 – 01/31/2021
Total Project Value	$ 250,000
Collaborator	Ohio State University
Technology Area	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.



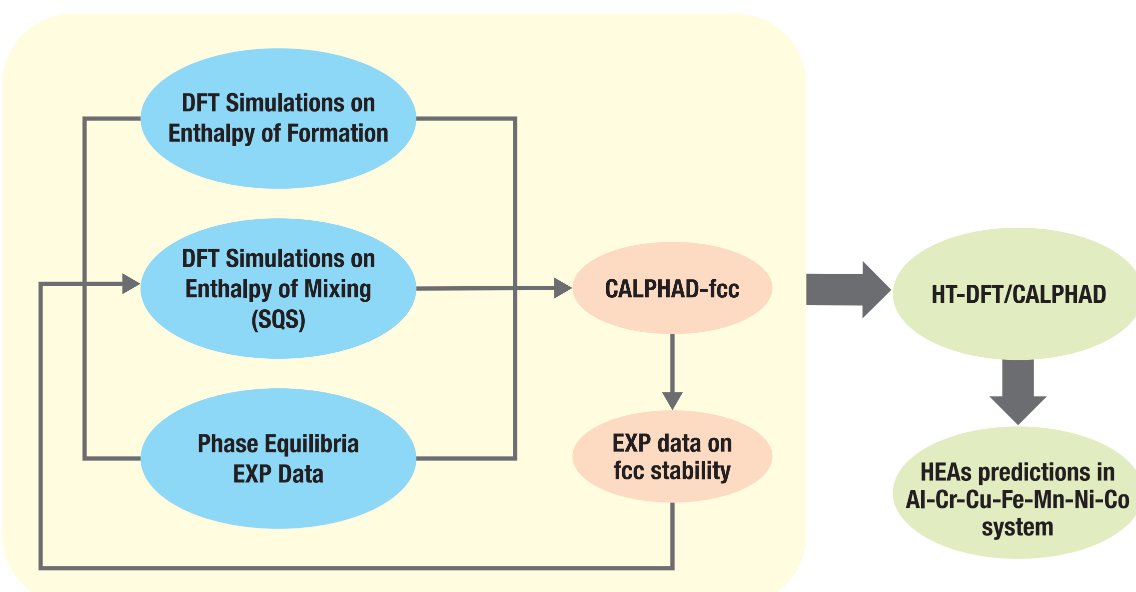
Materials design using ICME approach.

The Novel Hybrid Start-off Model of High Performance Structural Alloys Design for Fossil Energy Power Plants

Performer	**Florida International University**
Award Number	FE0030585
Project Duration	08/01/2017 – 07/31/2020
Total Project Value	$ 250,000
Technology Area	University Training and Research

The project team will develop an ab initio approach to quickly design new high-performance structural alloys for use in fossil energy power plants. The specific project objectives are to (1) conduct density functional theory (DFT) simulations for the selected Fe-Co-Cr-Ni quaternary system; (2) develop a thermodynamic database specifically for the face-centered cubic (FCC) phase of the selected system; (3) predict the compositions of new alloys in the selected system and compare them to experimental observations; (4) develop a hybrid high-throughput DFT/CALPHAD model capable of efficiently predicting the compositions of new alloys for multicomponent systems; and (5) apply the approach to make predictions on high-entropy alloys in an Al-Cr-Cu-Fe-Mn-Ni-Co multicomponent system.

The project will culminate in the development of a hybrid model based on high-throughput DFT simulations and computational thermodynamics to provide guidance on how to identify new multicomponent, high-performance structural alloys with much less computational effort. The model will address the extensive computational time needed for DFT when designing new alloys.



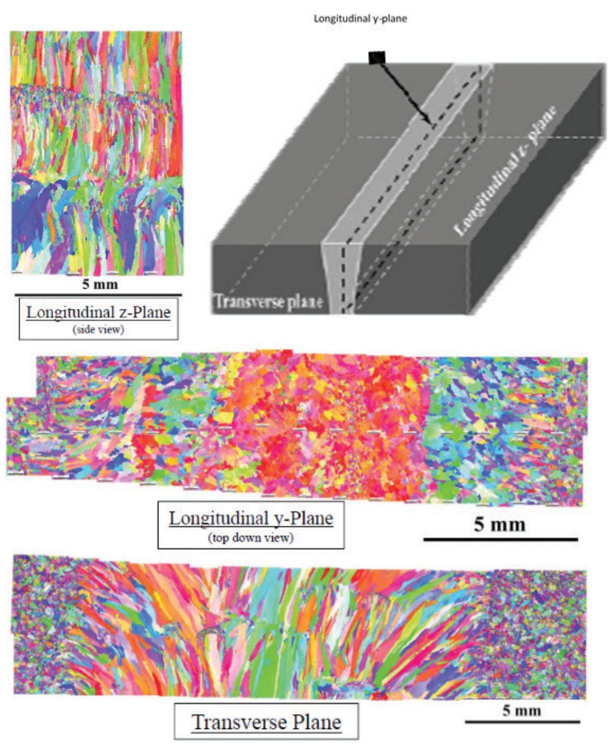
Development of the hybrid ab initio/CALPHAD approach.

Physics-based Creep Simulation of Thick Section Welds in High Temperature and Pressure Applications

Performer	**Idaho National Laboratory (INL)**
Award Number	FWP-B000-14029
Project Duration	06/01/2015 – 03/31/2020
Total Project Value	$ 955,000
Technology Area	Coal Utilization Science

Idaho National Laboratory (INL) will improve the capability to perform accurate and rapid computational modeling of the long-term mechanical behavior of nickel superalloy weldments that will be used in advanced fossil energy power cycles. An improved capability to predict the long-term behavior of weldments will allow materials scientists and structural component designers to optimize the use of advanced materials in advanced fossil energy applications. In this project INL will develop a microstructure-based creep model for nickel superalloys and add it to a computational platform, Multiphysics Object-Oriented Simulation Environment (MOOSE), that INL has developed for multi-scale simulation of the behavior of high-temperature materials in nuclear power plant applications.

This project will develop improved computational methods to predict the long-term behavior of advanced materials and structural components in fossil energy power plants that will reduce the time and expense of developing and qualifying new materials and enable a more cost-effective use of advanced materials at higher operating temperatures and pressures, which will result in higher-efficiency fossil fuel based power systems.



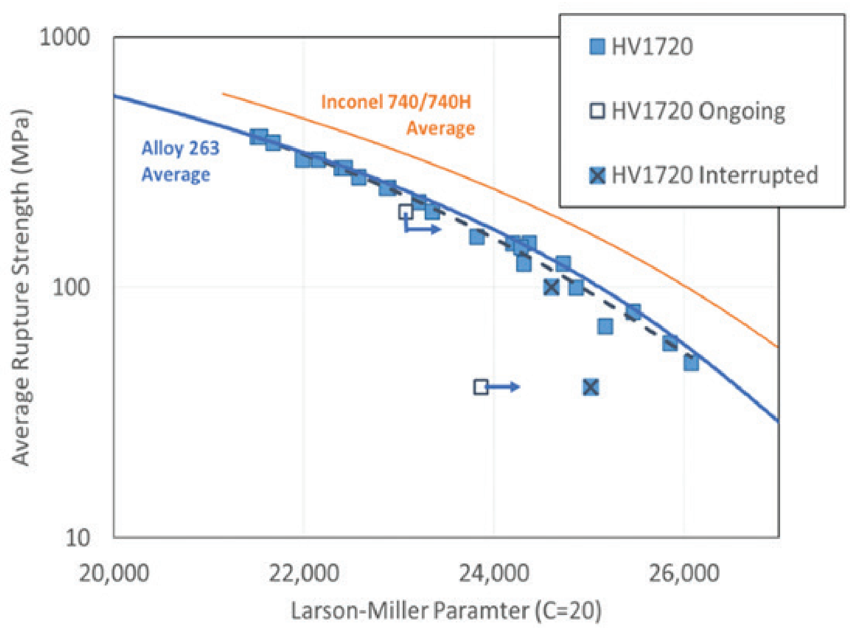
Microstructure of base metal, heat affected zone, and weld metal.

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

Performer	**Michigan Technological University**
Award Number	FE0027822
Project Duration	08/15/2016 – 08/14/2020
Total Project Value	$ 399,996
Technology Area	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 (γ') 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 (η) and gamma prime phases prior to creep testing, with the γ' 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 η + γ', and the Michigan Tech-modified Nimonic 263 alloy that contains only η); 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.



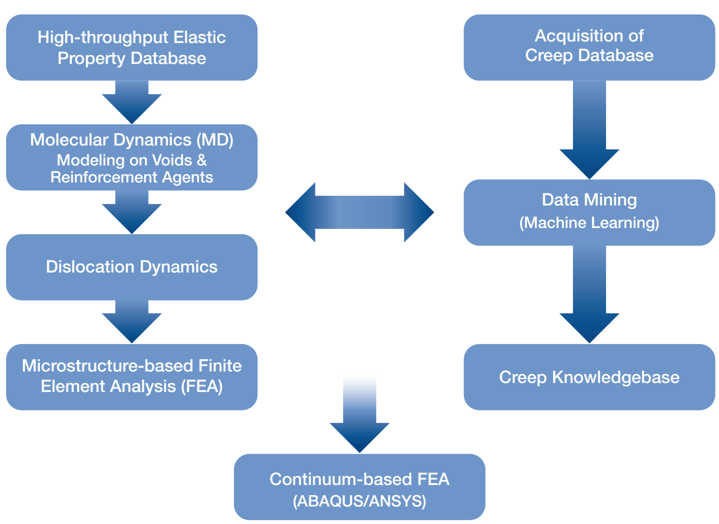
Alloy 20, Widmanstätten microstructure, creep.

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

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

NETL 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).

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	09/01/2017 – 09/30/2023	09/01/2017 – 09/30/2020	09/01/2017 – 09/30/2023	09/01/2017 – 09/30/2020	09/01/2017 – 09/30/2023	09/01/2017 – 09/30/2023	09/01/2017 – 09/30/2023
Funding to Date 09/01/2017-9/30/2021	$ 2,074,000	$ 981,000	$ 997,000	$ 590,000	$ 3,448,000	$ 2,604,000	$ 1,520,000
Total Project Value (All)	$ 9,610,000						
Technology Area	Coal Utilization Science						

Affordable, durable, heat-resistant alloys are necessary for improving the existing fleet of fossil energy (FE) power plants and enabling advanced fossil energy systems such as advanced ultra-supercritical steam cycles and supercritical carbon dioxide (sCO_2) power cycles. Advanced alloys will continue to be needed for FE plants of the future, flexible plants operating cyclically, as needed, at temperatures in excess of 700 °C (approaching 800 °C), and under complex mechanical loading conditions in harsh oxidizing environments for lifetimes exceeding 100,000 hours (12 years). 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.

The eXtremeMAT collaboration brings together leading national laboratories to harness the unparalleled breadth of unique capabilities across the DOE complex associated with materials design, high-performance materials computing, data science and analytics, manufacturing process development, basic and advanced materials characterization, and life cycle performance assessment into an integrated, mission-focused team, in order to revolutionize alloy development for fossil energy applications. Specifically, to:

- develop a suite of improved heat-resistant alloys for fossil energy components in existing and future power plants.
- improve models to predict long-term materials performance in existing and future fossil energy power cycles.

eXtremeMAT will achieve these goals by developing advanced physics-based, multi-scale computational models and simulations with machine learning approaches to more accurately predict performance under realistic service conditions. The technology breakthrough lies in the ability of these tailor-made models to predict the influence of initial microstructure on microstructural evolution and performance during component service. This approach constitutes a significant departure from existing empirically driven lifetime standards in which accuracy and sensitivity to microstructure and complex non-monotonic and non-uniaxial loading is either limited or altogether absent.

Over the last two years, eXtremeMAT has made significant progress on achieving its goals as follows:

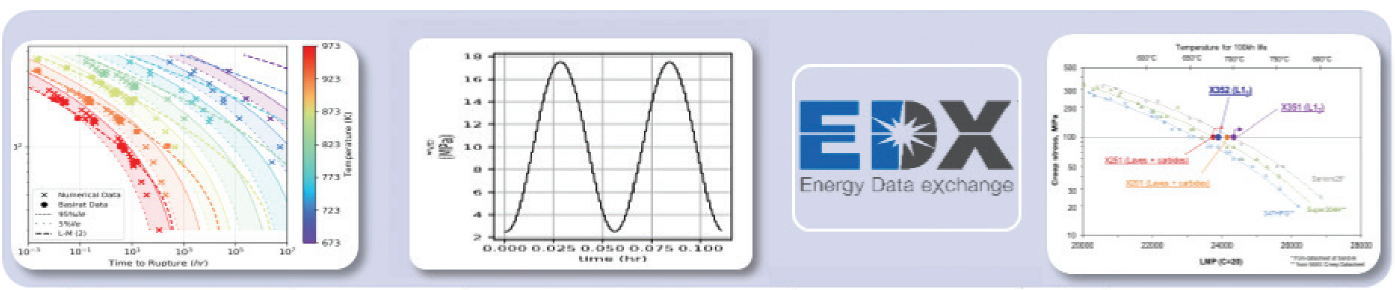
- A suite of eXtremeMAT models was developed to predict creep rupture life using a minimum of short-term creep tests. This model has been extended to multi-axial stresses and cyclic loading (i.e., ratcheting) conditions.

- A platform (database) is in place (on the NETL EDX site) to curate experimental and simulated data and metadata required for material data analytics in expediting design and development, as well as, material property life prediction.
- eXtremeMAT has accelerated the design of an alumina-forming alloy (AFA) with exceptional creep life compared to existing commercial alloys, e.g. 347H, Super 304H, and Sanicro25.

eXtremeMAT will demonstrate and deliver, by the end of project (September 30, 2023):

- **Alloy Lifetime Predictor:** A mechanistically based (i.e., physics and microstructure derived) multi-axial lifetime model for 347H and P91 steels. This model and its life prediction aspects will incorporate the complexities of stress loading, temperature, and microstructure.
- **Engineering Scale Lifetime Predictor:** A reduced order model for 347H stainless steel that can be implemented into commercial finite element codes. The tool will predict the performance lifetime of steel components subjected to multi-axial and cyclical loading and temperature in high-temperature steam environments, including mechanical and oxide spallation failure mechanisms.
- **Materials Database and Analysis Tools:** A curated database of experimental and simulation data for FE materials of interest. eXtremeMAT will also develop and demonstrate algorithms for automated detection of features in alloy microstructures that change with time, which can be used to predict how long a component may survive under differential operating conditions.
- **Accelerated Discovery of Alloys:** Demonstrate AFA stainless steels developed through the eXtremeMAT framework.

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



Material lifetime and performance predictors

Component lifetime and performance predictors

Materials database and analysis tools

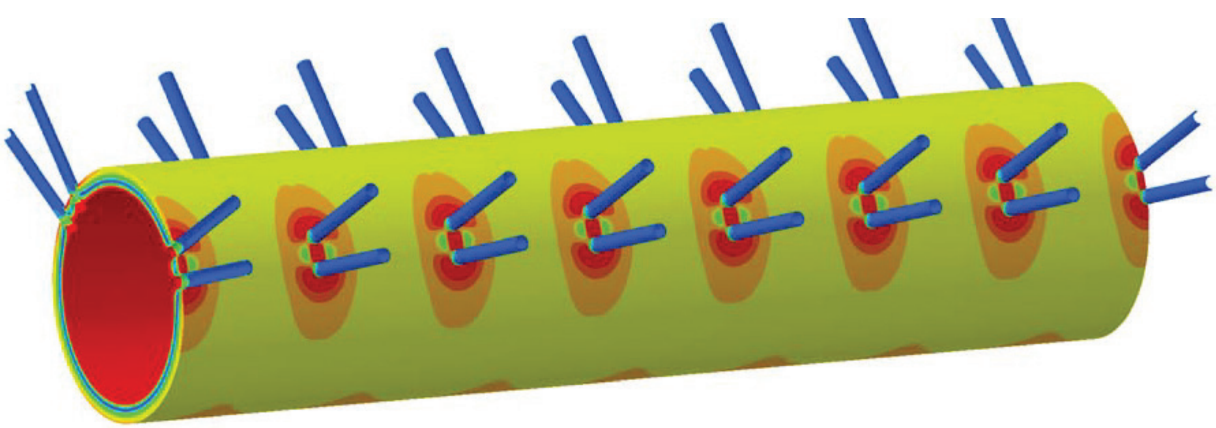
Rapid discovery of new alumina forming alloys

Alloy for Enhancement of Operational Flexibilty of Power Plants

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

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

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



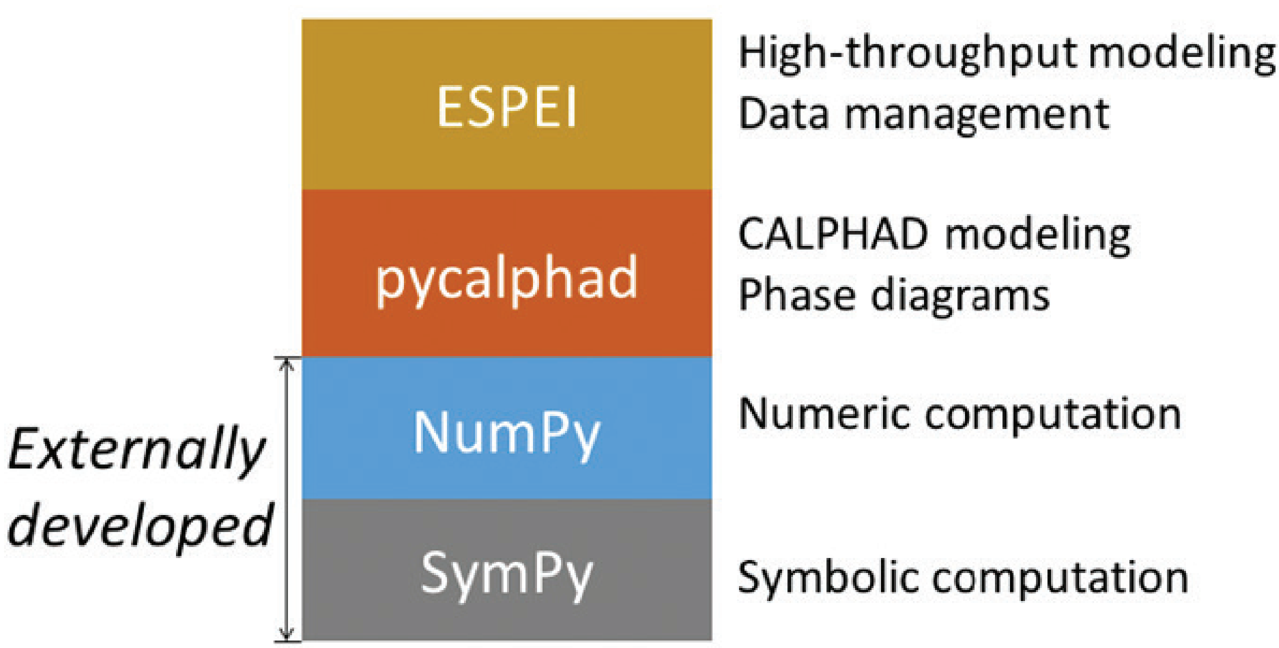
Stress contour plot of a steam header.

High Throughput Computational Framework of Materials Properties for Extreme Environments

Performer	**Pennsylvania State University**
Award Number	FE0031553
Project Duration	12/15/2017 – 12/14/2020
Total Project Value	$ 937,836
Technology Area	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.

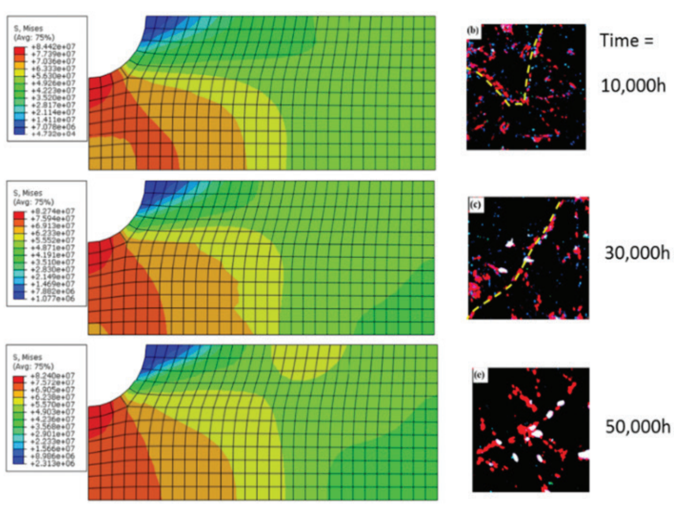


ESPEI-2.0 software stack.

Improved Models of Long-Term Creep Behavior of High Performance Structural Alloys for Existing and Advanced Technologies Fossil Energy Power Plants

Performer	**QuesTek Innovations, LLC**
Award Number	SC0015922
Project Duration	06/13/2016 – 01/31/2020
Total Project Value	$ 1,164,586
Technology Area	Plant Optimization Technologies

NETL is partnering with QuesTek Innovations LLC to develop a robust creep modeling toolkit to predict the long-term creep performance of materials for base alloys and weldments in fossil energy systems under wide thermal and mechanical conditions. Precipitation modeling using thermodynamic databases will provide fundamental quantities that will be used as inputs for upscaling strategies and methods. The goal is to establish microstructure-sensitive models that capture the different creep mechanisms observed in ferritic steels and integrate the models into QuesTek's Defense Advanced Research Projects Agency–Accelerated Insertion of Materials (DARPA–AIM) efforts to predict the variability of the creep strength as a function of the microstructure and service conditions. In the Phase I effort, the methods proposed have been demonstrated to predict creep life near 100,000 hours for P91 ferritic steels with microstructure inputs obtained from the National Institute of Material Science. In Phase II, the tools will be expanded and exercised in wider operating conditions including different temperatures and applied stresses in order to predict creep behaviors with over 300,000 hours creep life. Integration of precipitate evolution schemes into the long-term material behavior (i.e., stability of microstructure and the different phases over long periods), along with a refined uncertainty quantification of various material and process parameters, will be assessed and calibrated in Phase II. Additionally, the methodology that is developed would be applicable to alternative material systems and microstructures through additional modules that capture the relevant mechanisms of creep. Accurate and efficient quantification of material properties for advanced ultrasupercritical (AUSC) boilers will directly enhance the success of DOE's crosscutting research and new alloy development program and provide significant public benefits.



Model prediction with microstructure evolution.

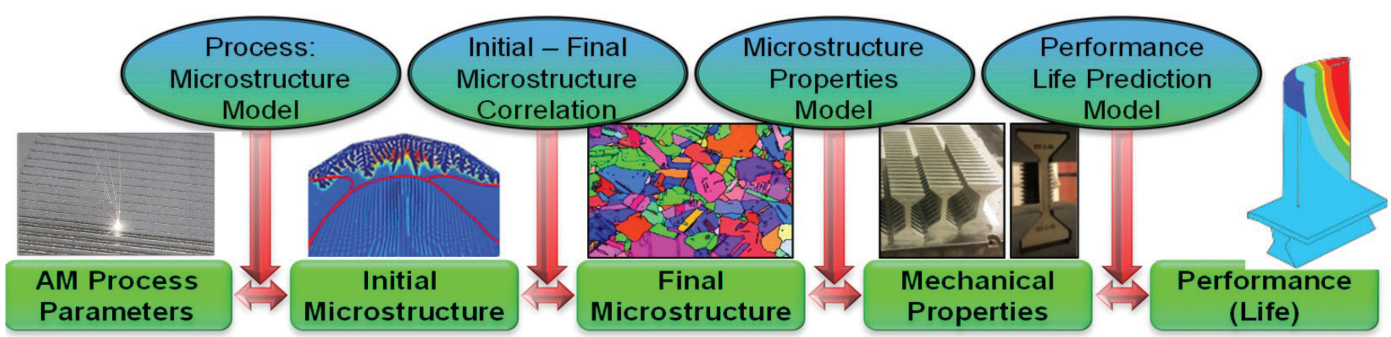
Computation Tools for Additive Manufacture of Tailored Microstructure and Properties

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

Raytheon Technologies Research Center (formerly United Technologies Research Center) is demonstrating the application of computational methods and tools on microstructure evolution and mechanical properties prediction for additively manufactured (AM) nickel-based superalloy parts. Models are being 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 is being demonstrated using these models. An integrated computational materials engineering framework that connects process, structure, properties, and performance is being 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.



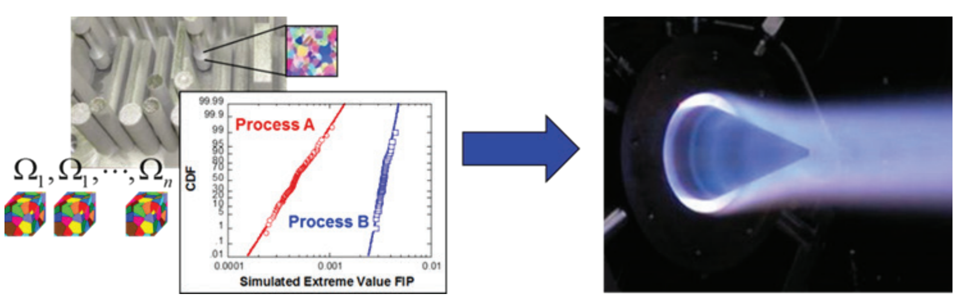
An ICME (Integrated Computational Materials Engineering) framework being developed by Raytheon Technologies Research Center that connects Process – Structure - Properties – Performance by four models.

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

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



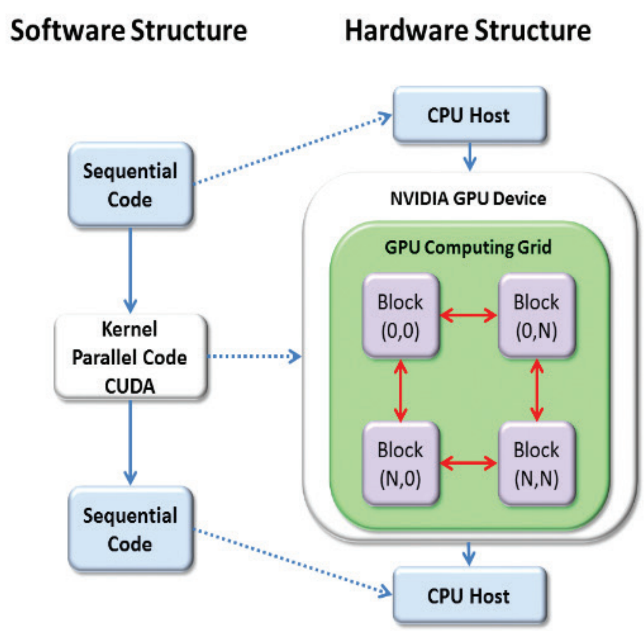
Modeling of additively manufactured parts leading to low-loss additively manufactured RDE injector.

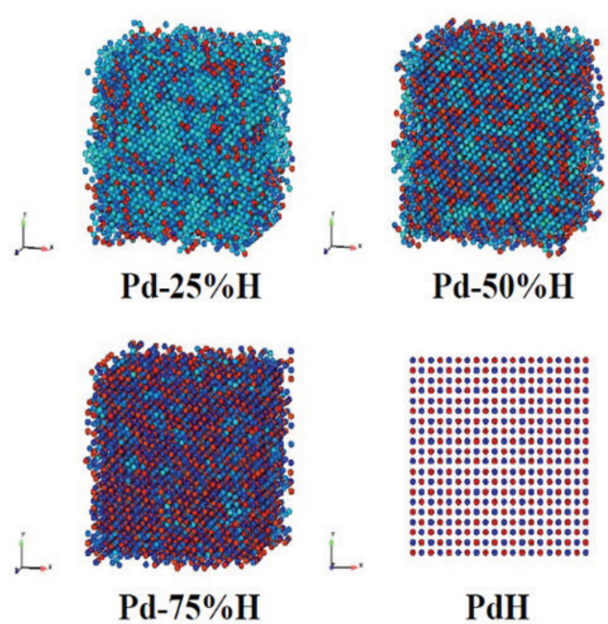
Large-Scale, Graphics Processing Unit (GPU)-Enhanced Density Functional Tight Binding (DFTB) Approaches for Probing Multi-Component Alloys

Performer	**University of California - Riverside**
Award Number	FE0030582
Project Duration	08/01/2017 – 06/30/2021
Total Project Value	$ 250,000
Technology Area	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.





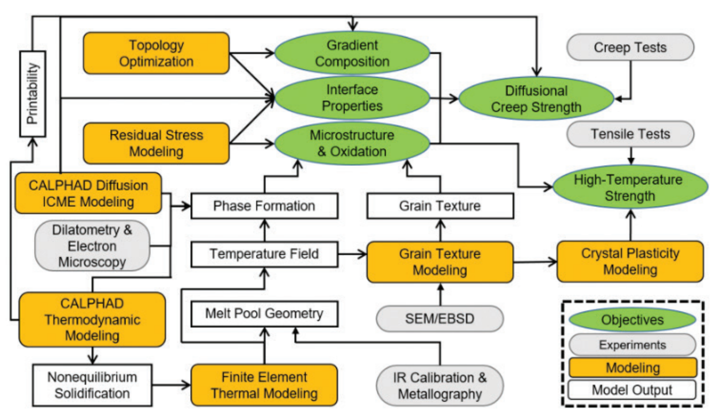
Large-scale simulations of alloy systems.

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

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

University of Pittsburgh (Pitt) researchers 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
°F .... degrees Fahrenheit
ACT .... accelerated creep testing
Al .... aluminum
AM .... additive manufacturing
AM-GCTJ .... additively manufactured graded composite transition joint
ASME .... American Society of Mechanical Engineers
AUSC .... advanced ultrasupercritical
CALPHAD ... calculation of phase diagrams (methodology)
CFD .... computational fluid dynamics
Co .... cobalt
CO_2 .... carbon dioxide
Cr .... chromium
CSEF .... creep strength enhanced ferritic
Cu .... copper
DARPA–AIM .... Defense Advanced Research Projects Agency–Accelerated Insertion of Materials
DFT .... density functional theory
DFTB .... density functional tight binding
DMW .... dissimilar metal weldments
DNV .... Det Norske Veritas
DOE .... Department of Energy
DofE .... design of experiments
DTMM .... digital twin material model
EEM .... extreme environment material
FCC .... face-centered cubic
FE .... Office of Fossil Energy
Fe .... iron
FSW/P .... friction stir welding and processing
FWP .... Field Work Proposal
GB .... grain boundary
GPR .... Gaussian process regression
GPU .... graphics processing unit
Gr.91 .... Grade 91
H282 .... Haynes 282
H_2O .... water
HBCU .... Historically Black Colleges and Universities
HIP .... hot isostatic processing
HP .... high-pressure
HPM .... High Performance Materials
HX .... Hastelloy X
ICME .... integrated computational materials engineering
ICWE .... integrated computational welding engineering
IN .... Inconel
IN740H .... Inconel 740H
INL .... Idaho National Laboratory
LP .... laser processing
MHD .... magnetohydrodynamic
Mn .... manganese
MOOSE .... Multiphysics Object-Oriented Simulation Environment
MPa .... megapascals
MWe .... megawatts electric
NETL .... National Energy Technology Laboratory
Ni .... nickel
NNS .... near net shape
O_2 .... oxygen (molecular)
ODS .... oxide dispersion strengthened
OMI .... Other Minority-Serving Institutions
ORNL .... Oak Ridge National Laboratory

ABBREVIATIONS

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_2.................................... 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

CONTACTS

Briggs White
Technology Manager
Crosscutting Research

412-386-7546

Briggs.White@netl.doe.gov

Patricia Rawls
Supervisor
Enabling Technologies and Partnerships Team

412-386-5882

Patricia.Rawls@netl.doe.gov

WEBSITES:

https://netl.doe.gov/coal/program124

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NATIONAL
ENERGY
TECHNOLOGY
LABORATORY

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

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

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

Program staff are also located in
Houston, TX and **Anchorage, AK**.

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