

Advanced Alloy Development Research



David Alman*, NETL, Research & Innovation Center

Crosscutting - High Performance Research Project Review Meeting (Virtual), June 3, 2021

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Advanced Alloy Development Field Work Proposal



Research Team

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Acknowledgement

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Program Focus*

- Robust domestic supply chain
- Prediction & Repair to manage flexible fleet of generators that enable high penetration of renewables into the grid
- Low-cost, high performance alloy development to enable the next generation Natural Gas Combined Cycle plants and the Hydrogen economy

*<https://netl.doe.gov/coal/high-performance-materials>

Advanced Alloy Development FWP

Affordable, Durable High-Performance Alloys.

- ✓ Techno-Economic & Market Assessments
- ✓ Alloy Development & Manufacturing
 - Simulate and Manufacture of Large-Scale Ingots
 - Cast Versions of Wrought Superalloys
 - Large Area Additive Manufacturing
 - Manufacturing of Compact Heat-Exchangers
 - Ni-, Fe- Alloy Development
- ✓ Materials Performance in Harsh Environments
 - Creep & Creep-Fatigue (LCF) modeling
 - Materials Performance in sCO₂ cycles

Presentations at Review Meeting

Advanced Alloy Development FWP



Tuesday, June 15, 2021

- 1:20 PM: Materials Performance in sCO₂ Environments, Omer Dogan
- 2:20 PM: Design Tool for Creep-Resistant Materials and Low Cycle Fatigue Modeling, Youhai Wen
- 2:40 PM: Simulate and Manufacture of Large-Scale Ingots & Summary of Past Ni-Alloy Development Work, Paul Jablonski

Eastern Daylight Time

Techno-Economic & Market Assessments

Research Guidance and Direction

Strategic Systems & Analysis Engineering

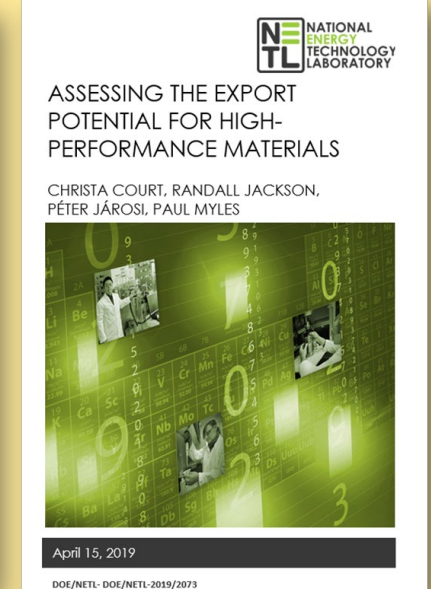
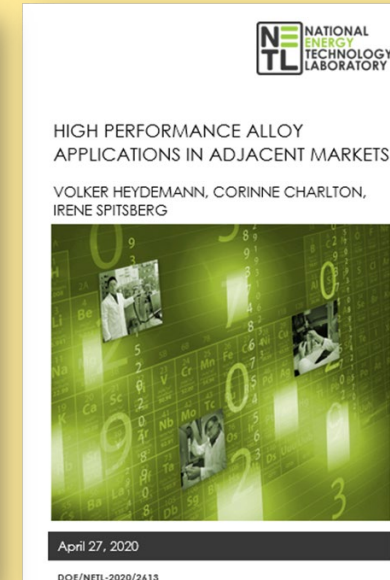
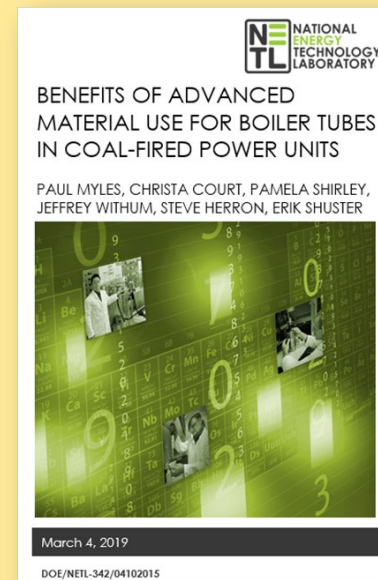
Previous Accomplishments

- High Performance Alloy Applications In Adjacent Markets
- Understanding the Supply Chain of Advanced Alloys
- Benefits of Advanced Materials for Boiler Tubes
- Export Potential for High-Performance Materials
- GADS Failures subsets analysis for boiler tubes, turbine, and balance of plant.

System Studies & Benefit Analyses

Reports on NETL's web site

<https://netl.doe.gov/crosscutting/publications>



Current Effort

Assessment of Advanced Alloy Opportunities for Natural Gas Combined Cycle (NGCC) Plants and H₂ Production

Identify how can advanced materials contribute to improved performance and reduced cost in NGCCs

- With and without CCS
- Interest in not only efficiency, but cyclability, reliability, service life, etc.
- Identify parameters of interest.
- Establish SOA design features, materials, and performance.
- **Identify materials-driven opportunities for improvement - informed by literature and consultants.**

Contact: Travis Shultz (travis.shultz@netl.doe.gov)



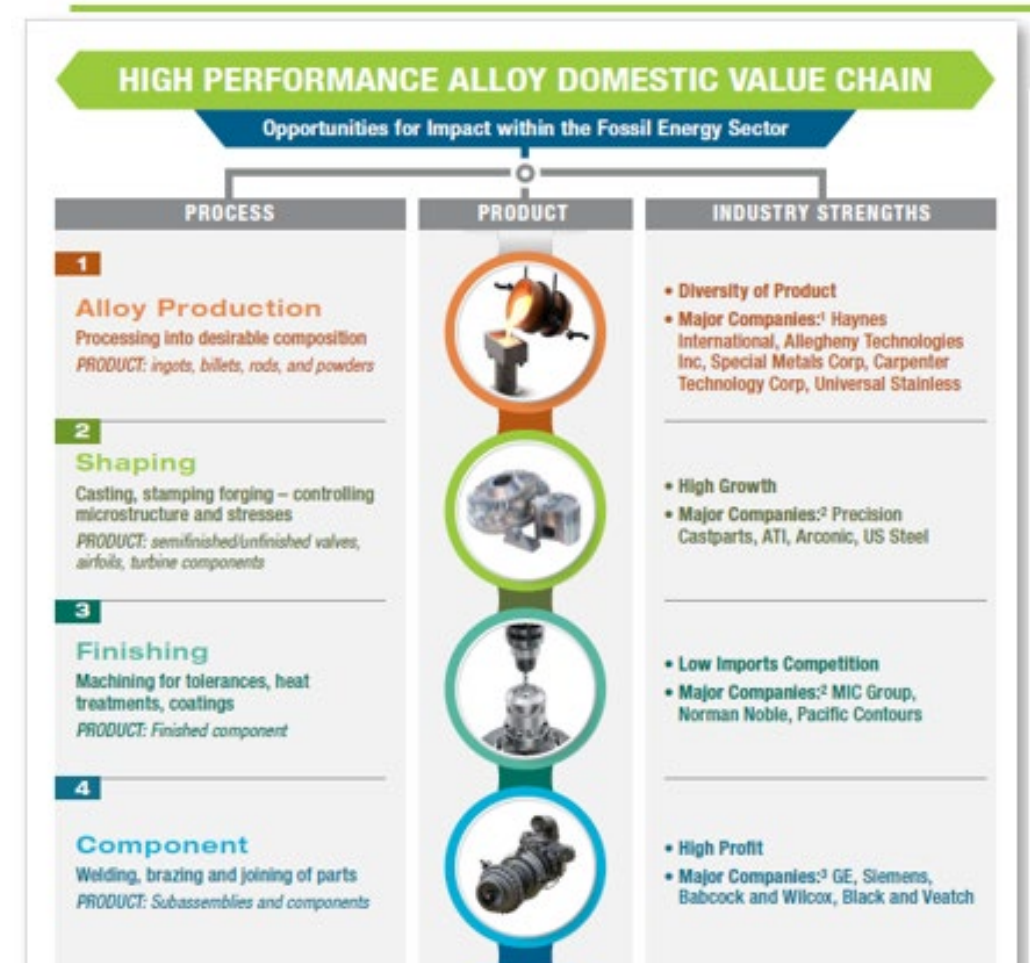
Current Effort

Benefits, Advantages, and Opportunities for Cost Reduction in the Materials Value Chain From Advanced Manufacturing for Power Plant Applications

Assess the economic benefit of novel manufacturing approaches in production of key, cost-driving components of the advanced power system and identify R&D challenges to realizing these benefits.

- Explore the most rapid path to market being used in current AUSC designs
- Investigate near-net-shape manufacturing techniques to reduce post-processing of large cast parts
- Study manufacturing one-off parts, reducing inventory, reducing wait times, and modification of larger parts in power plants

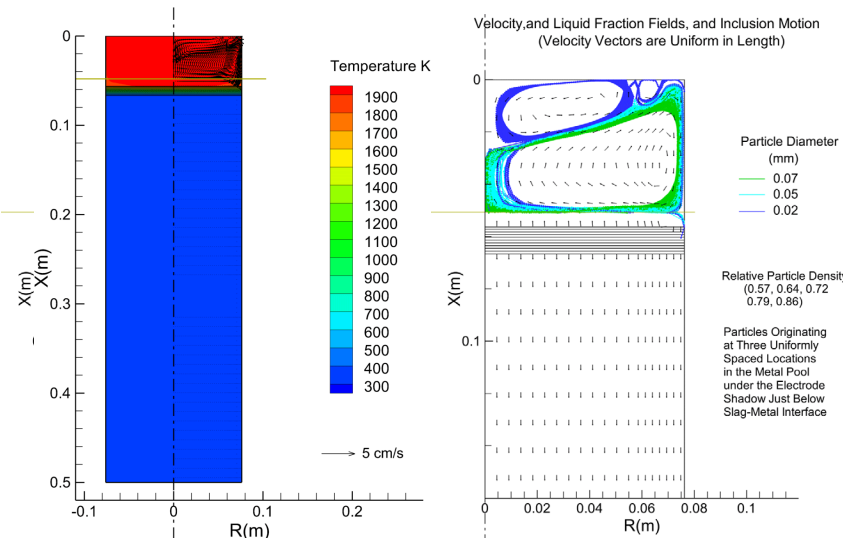
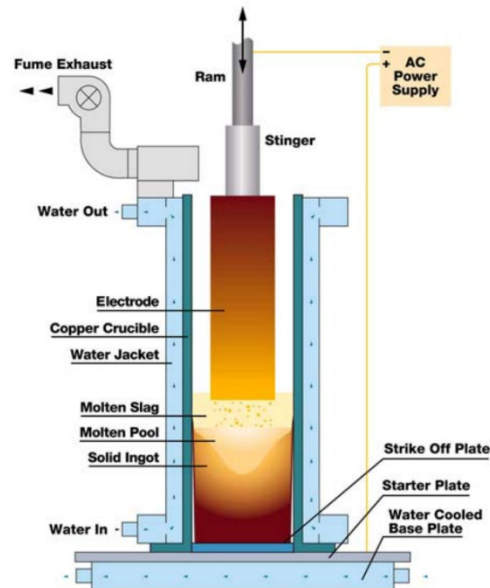
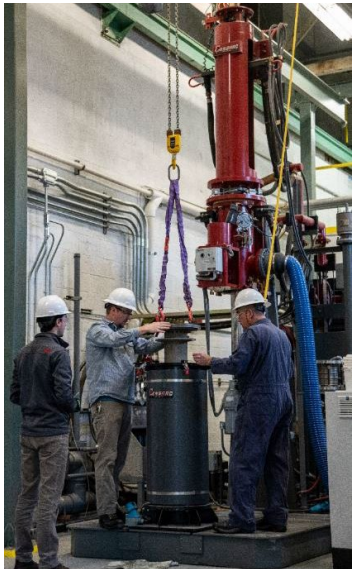
Contact: Erik Shuster (erik.shuster@netl.doe.gov)



Simulate & Manufacture of Large-Scale Ingots

Improve Electro-slag-remelting (ESR) ingot quality & melt efficiency.

- Optimize melt parameters (and alloy/slag compositions) to maximize ingot quality.
- *ESR used for mission critical applications*
- Combine CFD (MeltFlow) & CALPHAD (JMatPro, Thermo-Calc) methods with experiments.
- Methodology to predict segregation during ESR melting as a function of process parameter (such as slag temperature, melt rate, fill factor). Important for alloy element retention and control of tramp elements.



By applying models:

- ✓ Improved yield during ESR melting of NETL Fe-9Cr alloys (CPJ7, JMP) XMAT alloys (347).
- ✓ Achieved 41% reduction in power required to melt at constant melt rate for master alloy production.
- ✓ Reduced tramp element concentrations in ESR ingots.
- ✓ Controlled chemistry for elements in tight concentration ranges.

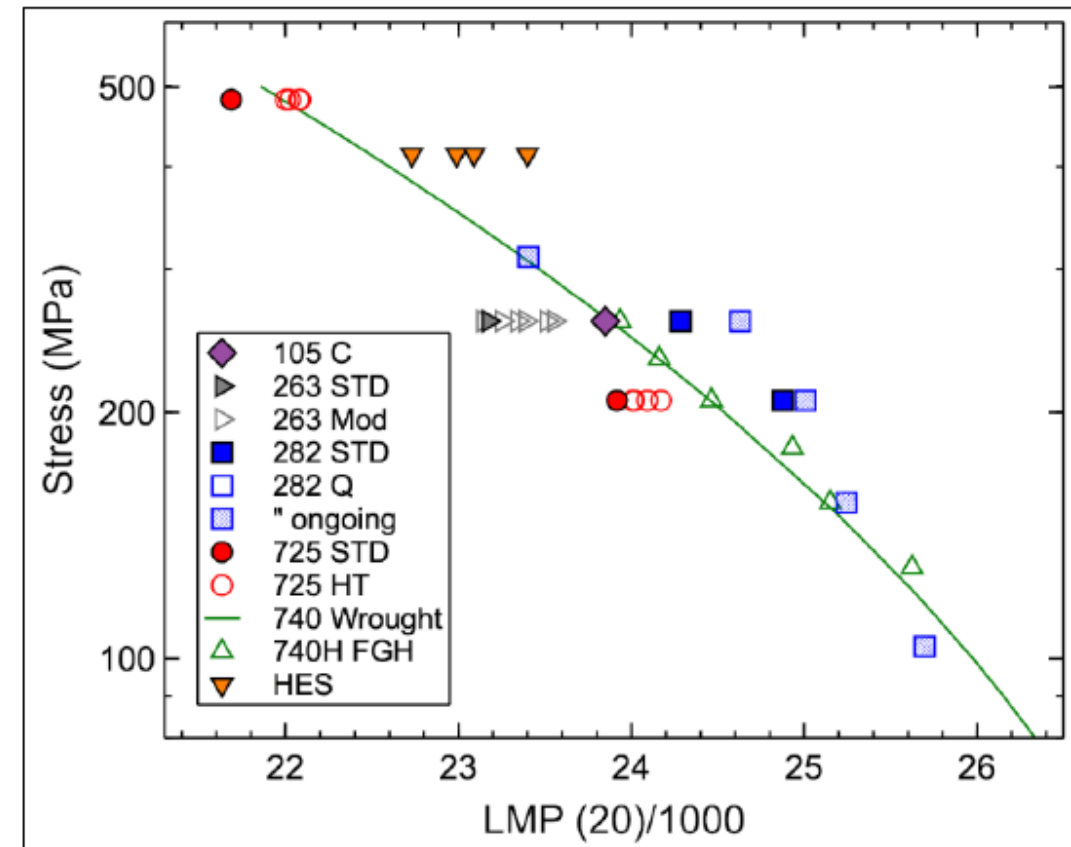
Contacts: Paul Jablonski (paul.jablonksi@netl.doe.gov) Martin Detrois (martin.detrois@netl.doe.gov)

Current Effort

Apply models to Ni-superalloy melting & upscaling

- Emphasis on NETL developed Ni-superalloys – large range of chemistries & microstructures.
- Provides insights on processability of superalloys (pre-competitive).
- Increase the likelihood of transfer to U.S. industry

Creep of NETL Superalloys compared to wrought 740H



Contacts: Paul Jablonski (paul.jablonksi@netl.doe.gov) Martin Detrois (martin.detrois@netl.doe.gov)

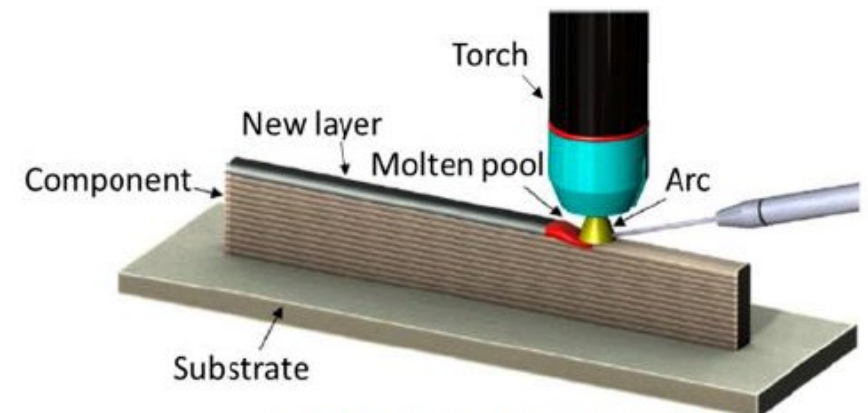
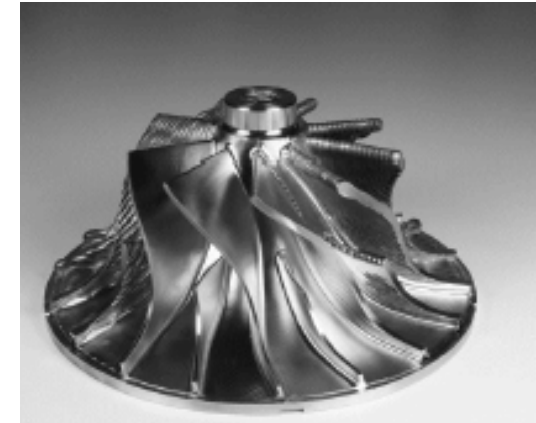
Large Area Wire Arc Additive Manufacturing

Identify the technical research challenges and opportunities for LA-WAAM and other wire-based AM methods for the production, repair, and **alloy feedstock development of precipitation strengthened superalloys.**

Current Effort

Gap Analysis for Feedstocks for LA-WAAM

- Establish an industrial technical committee that actively contributes feedback to gap analysis
- Develop research road map

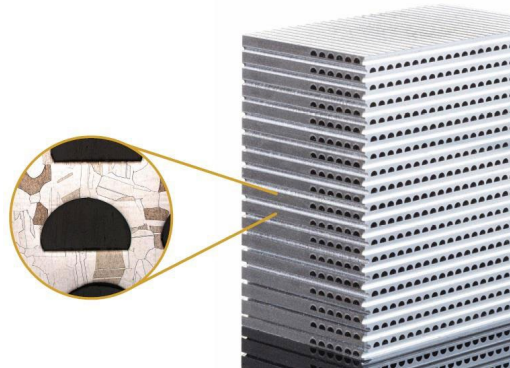
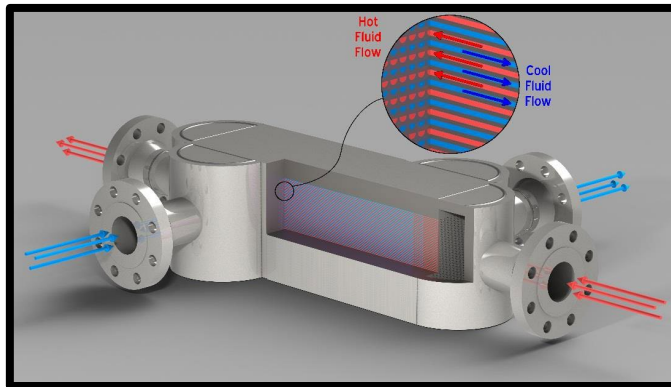


T.A. Rodrigues, Materials. 12 (2019).
<https://doi.org/10.3390/ma12071121>.

Contact: Chantal Sudbrack (chantal.sudbrack@netl.doe.gov)

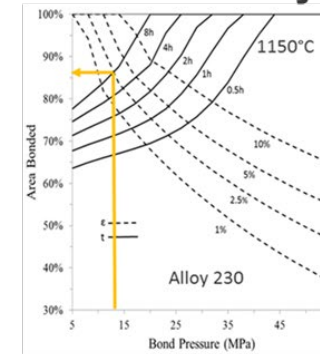
Manufacturing Compact Heat Exchangers

- sCO₂ power cycles – highly recuperated cycle
- sCO₂ power cycle conditions necessitate the use of higher temperature materials
- **Demonstrate a diffusion bonding process in accordance with Appendix 42, ASME Section VIII, DIV 1 for Alloy 740H**

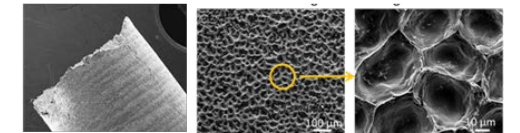
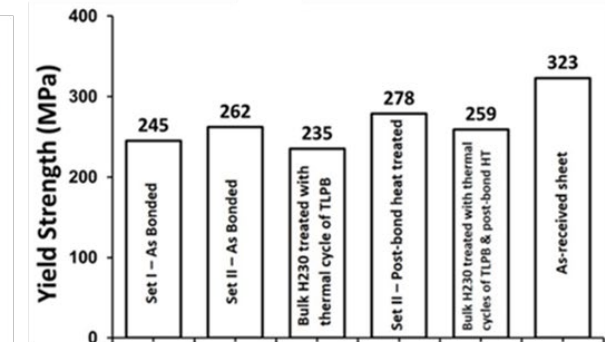
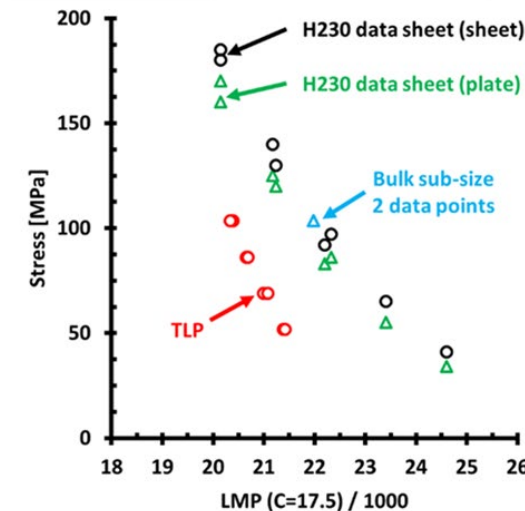
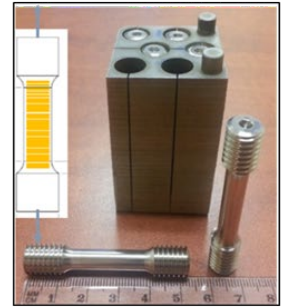


Prior research on Alloy 230

Transient-liquid-phase (TLP) bonding using Ni-P interlayers developed for Alloy 230.



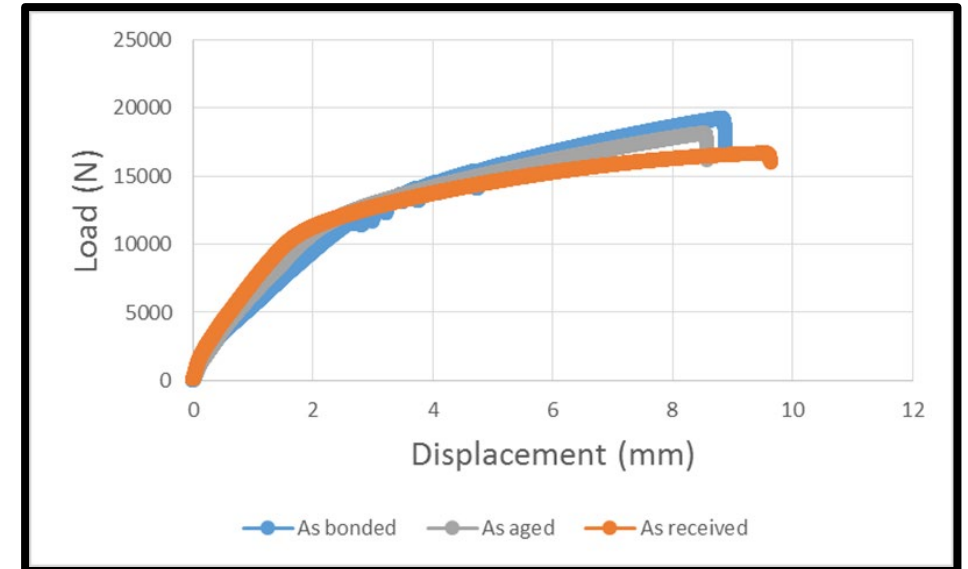
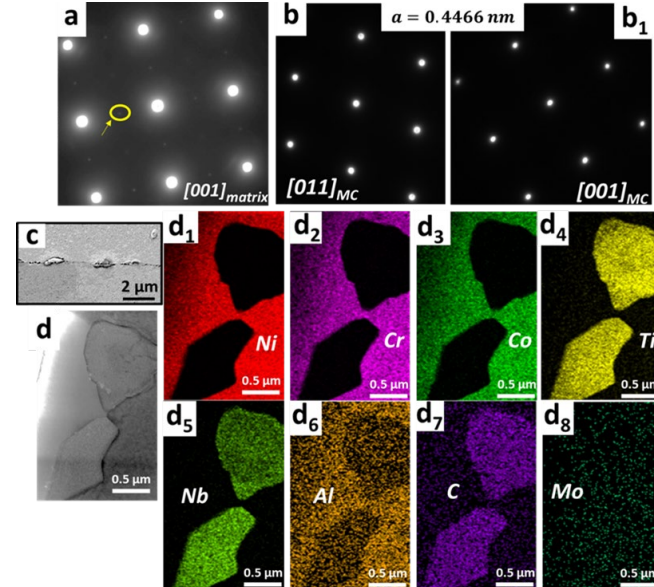
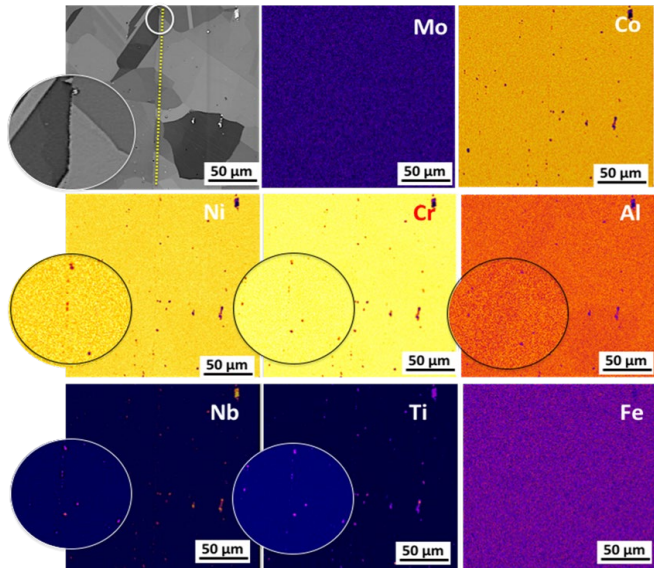
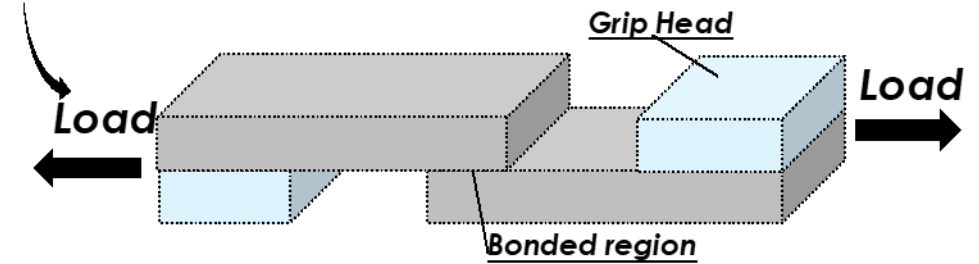
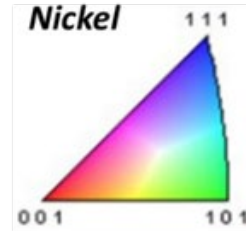
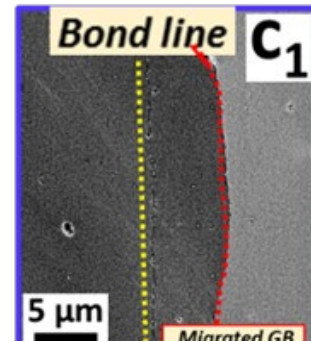
Strength of the bonded stacks was greater than 85% of base alloy 230 yield stress. Bonded stacks possessed acceptable low-cycle fatigue and creep properties. However, plastic strain localization in the bond region caused low tensile and creep elongation



Contact: Omer Dogan (omer.dogan@netl.doe.gov)

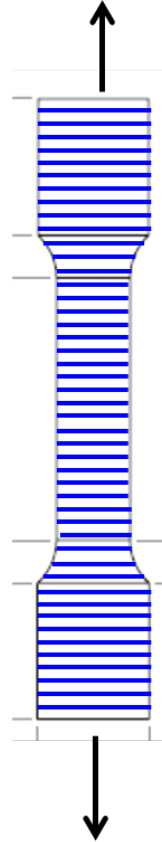
Manufacturing Compact Heat Exchangers

Demonstrated diffusion bonding of 740H



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Manufacturing Compact Heat Exchangers



Current Effort

Demonstrate a diffusion bonding process for IN740H in accordance with Appendix 42, ASME Section VIII, DIV 1.

- Produce diffusion bonded stacks of 50 sheets
- Tensile yield stress and elongation > 75% of the bulk material.

Acknowledge the collaboration of:



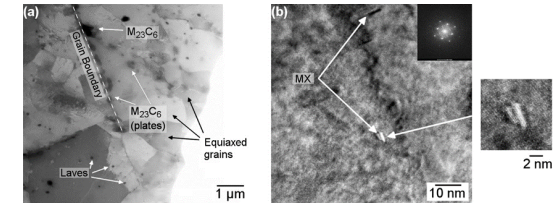
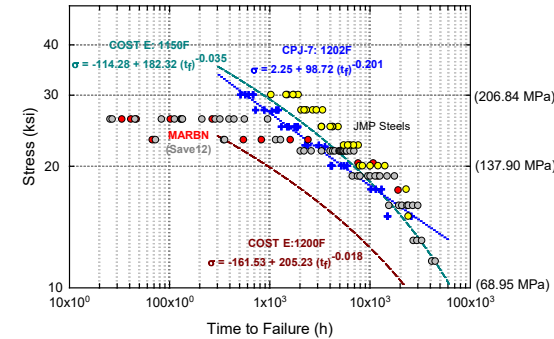
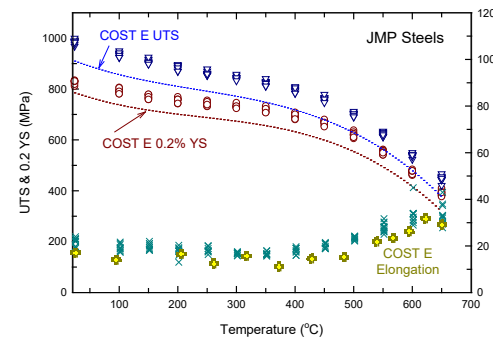
Contact: Omer Dogan (omer.dogan@netl.doe.gov)

650°C Martensitic-Ferritic Steel Development

Improve the temperature capability and performance life of the relatively low-cost Fe-9–12% Cr ferritic-martensitic steel.

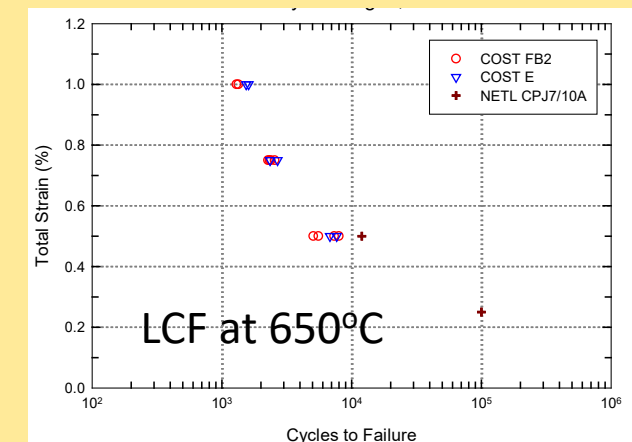
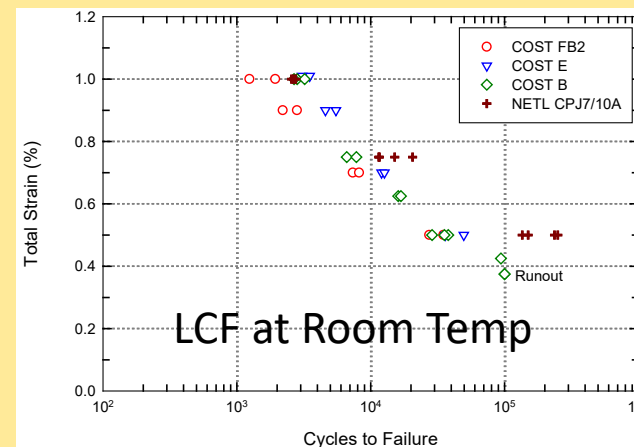
NETL-CPJ7 and NETL JMP Steels

- ★ Cast and wrought forms
- ★ 70kg (150 lb) ingots produced and reduced to plate (VIM, ESR)
 - Formulated ESR slag chemistry
- ★ Welding trials/studies
 - Conventional NETL
 - Friction Stir Welding PNNL
- ★ Material available for evaluation



Current Effort

✓ Low cycle fatigue (LCF), Hold-time fatigue, and Project

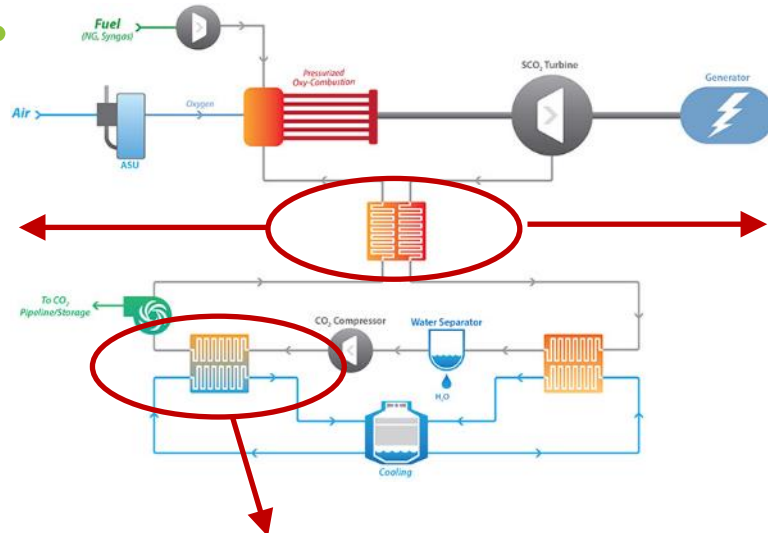
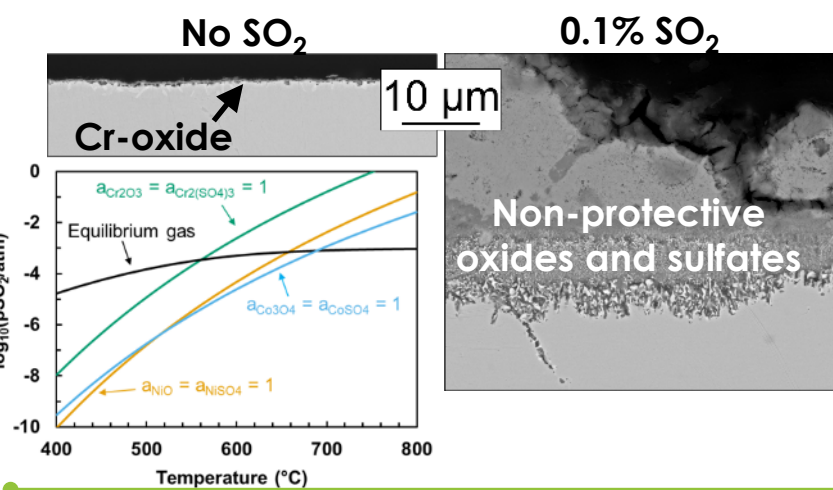


Contact: Jeffrey Hawk (jeffrey.hawk@netl.doe.gov)

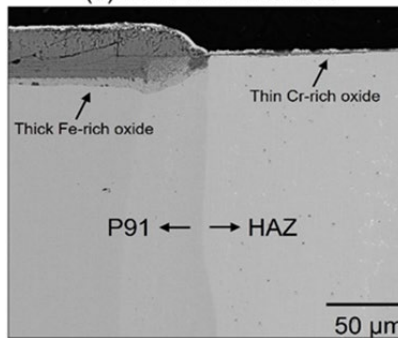
Materials Performance in Supercritical CO₂ Power Cycles

HIGH-TEMPERATURE OXIDATION OF STEELS AND SUPERALLOYS

Effects of impurities and pressure



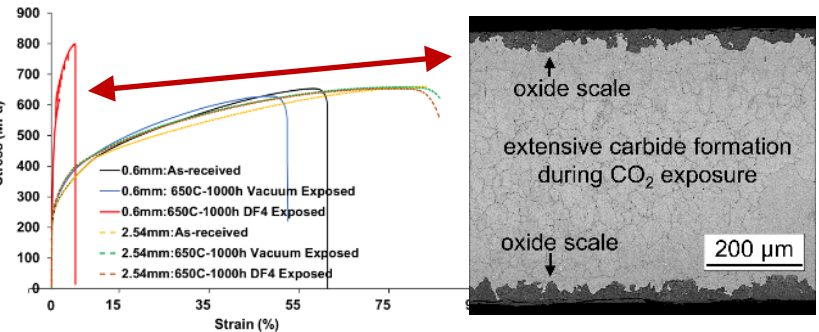
JOINING



Dissimilar metal welds investigated

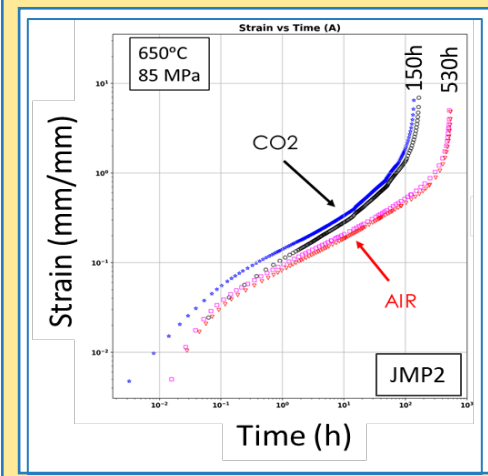
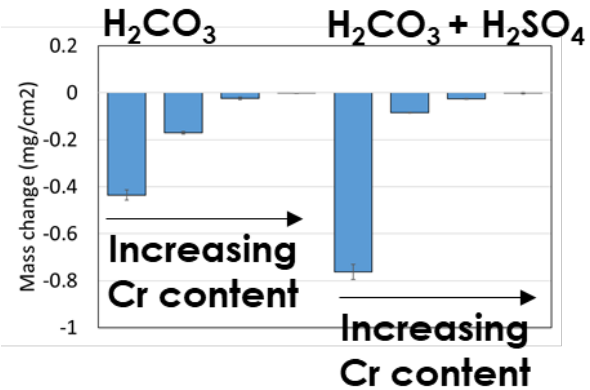
- P22-P91
- P91-347H
- P22-Alloy 263
- Alloy 625-Alloy 263
- 347H-Alloy 263

LINKING OXIDATION BEHAVIOR AND MECHANICAL DEGRADATION



LOW-TEMPERATURE CORROSION

Identifying low-cost steels resistant to acidic condensates



Current

Effort

Impact of CO₂ on:

✓ creep

✓ creep-fatigue

Contacts: Omer Dogan (omer.dogan@netl.doe.gov), Richard Oleksak (richard.oleksak@netl.doe.gov)

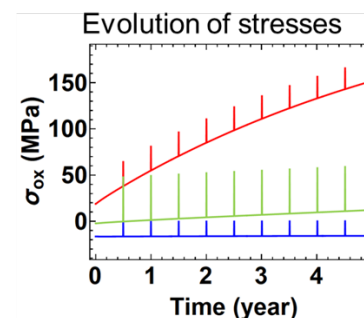
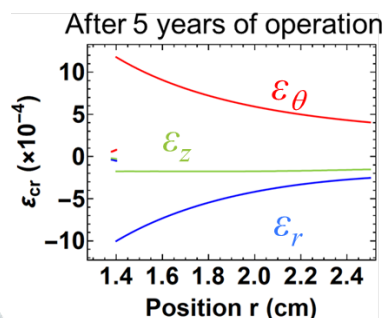
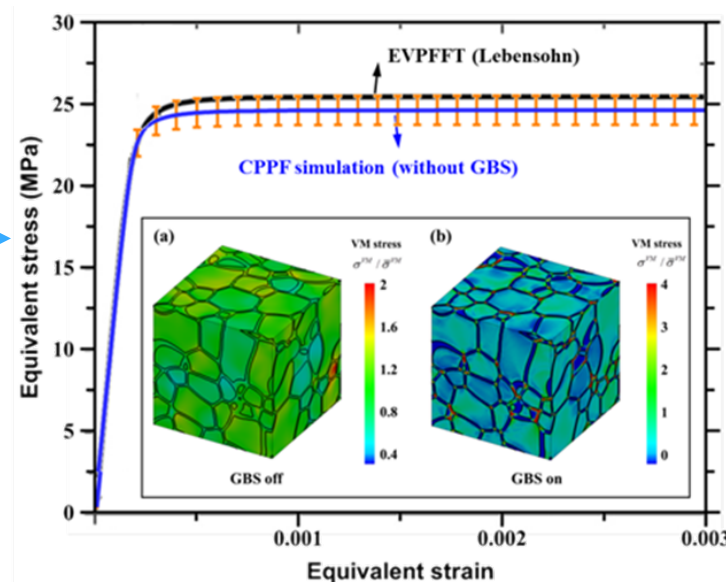
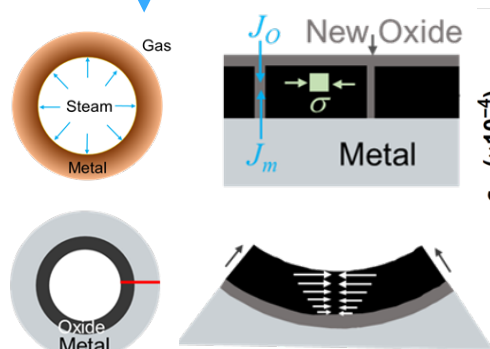
Creep & Creep-Fatigue (LCF) modeling

Develop a microstructure-based life prediction tool that couples creep, fatigue, and environmental effects.

- Developed a crystal plasticity phase-field model that includes both shear deformation in each slip system of polycrystals and grain boundary sliding (GBS).
- Developed a phase-field model of precipitation process with continuous coherency loss.
- Developed a microstructural based oxide-scale spallation model

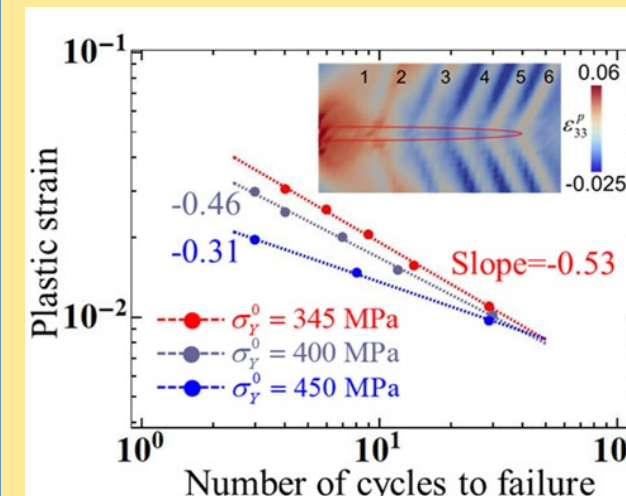
Spallation due to:

- Temperature (Different thermal expansion)
- Oxide growth strain with geometric constraint
- Different creep rate between oxide and metal



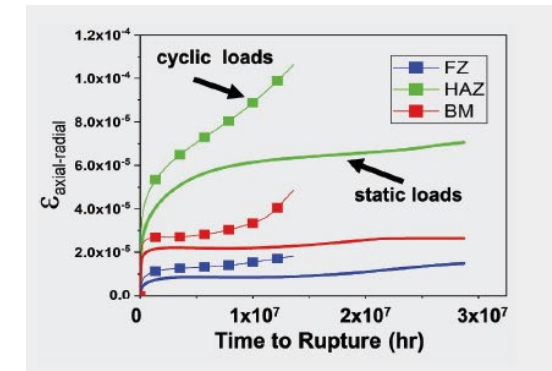
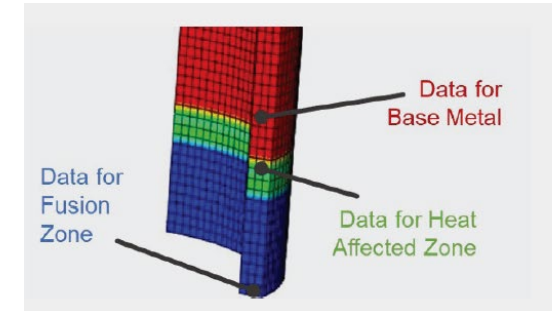
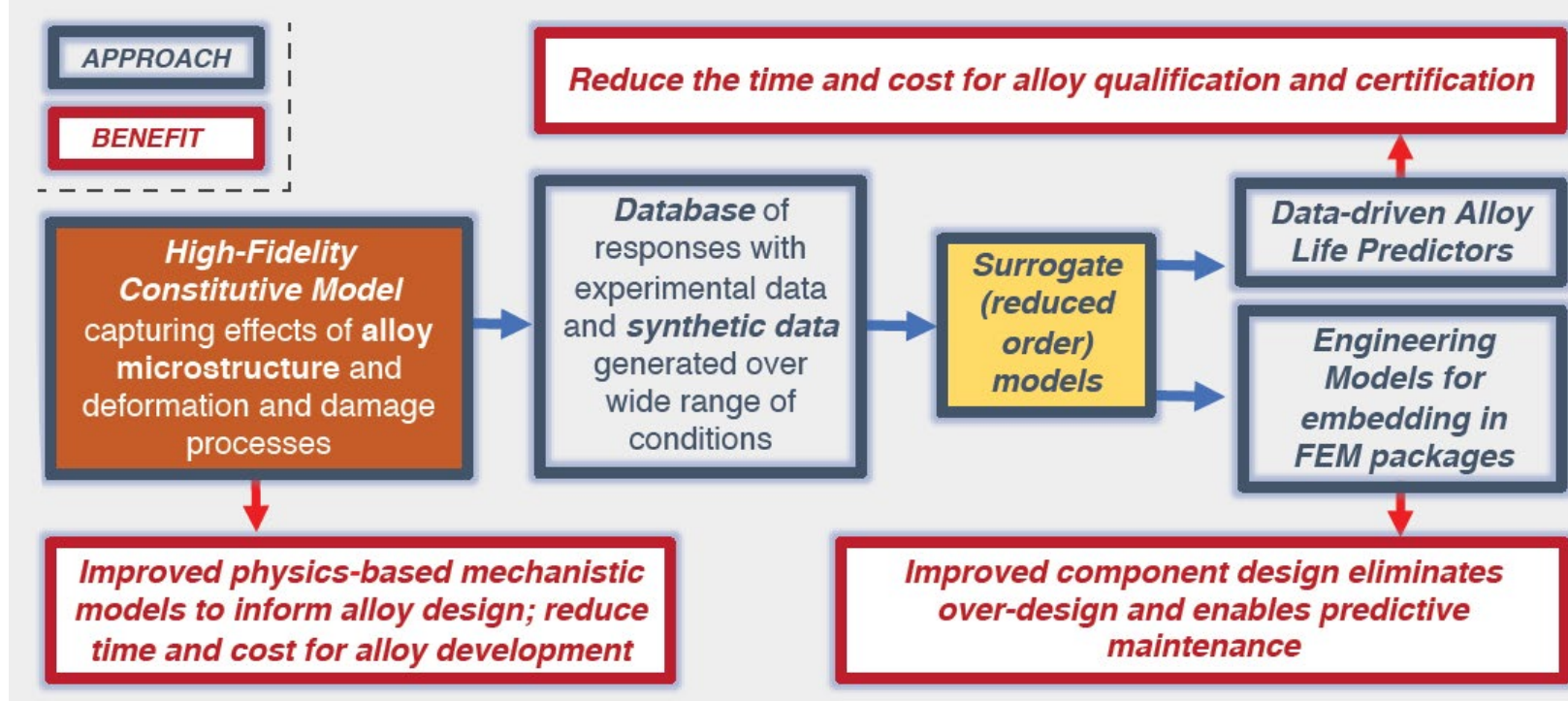
Current Effort: LCF modeling

Phase field model
to predict the LCF



Contact: Youhai Wen (youhai.wen@netl.doe.gov)

eXtremeMAT



- Tuesday, June 8, 2021, 11:10 AM (EDT): eXtremeMAT Computational Simulations Laurent Capolungo (LANL)
- Tuesday, June 15, 2021, 1:20 PM (EDT): eXtremeMAT Guidelines for Alloy Development Edgar Lara-Curzio (ORNL) & Jeffrey Hawk (NETL)

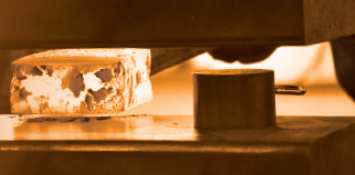
Visit Us At

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NETL's

Advanced Alloy Development Research



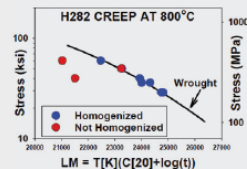
NETL utilizes an integrated alloy development approach that leverages computational materials engineering, manufacturing at scale, and performance assessment at condition to develop alloys solutions to enable advanced technologies.

NETL has demonstrated and deployed alloys with improved performance capabilities for energy applications, aerospace, defense, and bio-medical applications. NETL has also implemented technologies to improve melting and casting practices.

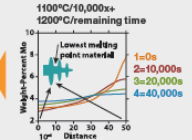
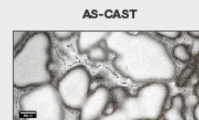
NETL's Award Winning Computational Homogenization Heat Treatments Routine

NETL has developed a computational routine to homogenize castings and ingots. The approach uses CALPHAD and simulations of the diffusion of alloying elements based on measured or calculated dendrite arm spacing from a casting to devise multi-step heat-treatments to homogenize alloy castings. The NETL methodology won an R&D 100 award in 2016.

The technology was developed to demonstrate that thick wall castings could be manufactured from typically wrought gamma-prime strengthened Ni-base superalloys. NETL demonstrated that through proper homogenization, cast alloys could be produced that have equivalent creep properties to the wrought versions of the alloy. This was key in enabling Advanced Ultra-Supercritical Steam (A-USC) turbine technology (A-USC). In support of the A-USC program, NETL designed heat-treatments of subsequently larger ingots and castings that were produced at a variety of commercial casting and heat-treating facilities. This culminated with the design of a heat-treatment for an 1/2 valve body 18,000-pound demonstration casting of a precipitation hardened superalloy. One aspect of the NETL routine, is that heat-treatments can be tailored to meet existing furnace capabilities available at the heat-treating facility.



Creep properties of alloy H282 in cast and wrought form. Properly homogenized casting have equivalent properties to wrought alloy.



www.netl.doe.gov

REFERENCE:
Jablonowski, P.D. and J.A. Hawk, Homogenizing Advanced Alloys: Thermodynamic and Kinetic Simulations Followed by Experimental Results. Journal of Materials Engineering and Performance, 2017, 26(1): p. 4-13.



NETL's

Advanced Alloy Development Capabilities



ALLOY FABRICATION CAPABILITIES

Melt Processing Capabilities

- Air Induction Melting: up to 300 lbs.
- Vacuum Induction Melting: 10, 50, and 300 lbs.
- Vacuum Arc Remelting, Electro Slag Remelting: 3- to 8-inch diameter ingots, 50-500 lbs.
- Button Melting: 50-500 grams



Heat Treatment & Fabrication Capabilities

- Heat-treatment furnaces: 1650°C, inert atmospheres and controlled cooling
- Press Forge: 500 Tons
- Hot and Cold Roll mills: 2 and 4 high configurations



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NETL's

Materials Performance Capabilities



Laboratory Capabilities to Simulate Real World Environments

Severe Environment Corrosion/Erosion Research Facility (SECERF)

Modular facility that allows researchers to examine the performance of materials under a wide variety of corrosion and hot-corrosion conditions, such as "fire-side" power generation conditions.

- Provides the basic infrastructure for conducting experiments at varying temperatures, in pure or mixed-gas environments, and in pure- or mixed-gas/liquid environments
- Available gases: CO, CO₂, CH₄, H₂, H₂S, SO₂, HCl, O₂, N₂, Ar, He, air, H₂O vapor
- Gas flow rates: 5-4000 mL/min
- A programmable gas delivery system with mass flow controllers, monitors, and interlock system allows for safe 24/7 unattended operations
- Temperature Range: Furnaces – Ambient to 1600°C; Hostile Atmosphere Erosion testing apparatus – Ambient to 900°C



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Corrosion & Oxidation Laboratories

Capabilities include systems for steam exposures, supercritical CO₂ exposures, and high pressure/high temperature immersion tests involving saturated CO₂ or mixed gas involving Air, Ar, N₂, CO₂, O₂, SO₂, H₂S, CH₄, NH₃.

- Ultra-super-critical (USC) Steam Autoclave: Dual rated to 4500 psig at 760°C and to 5000 psig at 746°C
- Supercritical CO₂ Autoclave: Rated – 4000 psig at 800°C
- Autoclaves for immersion testing in saturated CO₂ or mixed gas involving Air, Ar, N₂, CO₂, O₂, SO₂, H₂S, CH₄, NH₃; Standing Stirred Autoclaves (5000 psig, 250°C), Flow-Through Unit (5000 psig, 500°C)
- Available static and cyclic oxidation testing for 24/7 exposures to: air, O₂, N₂, Ar, He, CO₂, H₂O, and N₂/4% H₂ at ambient and elevated temperatures
- Electronic potentiostats/galvanostats for conducting electrochemical experiments
- Capabilities to perform electrochemical experiments at high-pressures and temperatures (4500 psig, 250°C) in in saturated CO₂ or mixed gas involving Air, Ar, N₂, CO₂, O₂, SO₂, H₂S, CH₄, NH₃

Fracture Mechanics & Creep Capabilities

- Mechanical Testing: tension, compression, low and high cycle fatigue, fatigue crack growth rate testing using electro-mechanical and servo-hydraulic Universal Testing Machines (5,500 to 220,000 lbs.) with high temperature capability and with fully instrumented computer control and data acquisition.
- Creep Testing: creep frames for stress-rupture and creep-rupture tests and stress relaxation tests. Testing can be done in Air, Ar, CO₂, or N₂. Maximum load capacity of 10,000 lbs. and a maximum temperature capability of 1200°C.

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