Advanced Materials Development FWP (#1022406)



Ömer Doğan, Technical Portfolio Lead





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Hydrogen Production w/CCS and Hydrogen Utilization



- Advanced Materials Development for Hydrogen Service
 - Environmental Barrier Coatings (EBCs) for Ceramic Matrix Composites (CMCs) in hydrogen turbines
 - Steels for high-temperature hydrogen service
 - Transformational high-temperature (850–1,000°C) Ni-based superalloys
- Advanced Manufacturing of Structural Materials
 - Robust domestic high performance alloy supply chain
 - Reduce the costs of Ni-based super alloys and enhance cyclic capabilities of materials
 - Cost-effective manufacturing and performance optimization of hydrogen resistant superalloys through Wire-Arc Additive Manufacturing (WAAM)
- Performance of Advanced Materials for Advanced Energy Systems
 - Impacts of hydrogen on materials performance and safety
 - Design tool for life prediction of CMCs and T/EBCs in hydrogen turbines
 - Expand performance prediction tools to hydrogen effects



Environmental Barrier Coatings for Protection of Ceramic Matrix Composites in Hydrogen-Based Turbines

Design and Evaluation of Environmental Barrier Coatings for Protection of Ceramic Matrix Composites in Hydrogen-Based Turbines

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Objective: Design and validate environment barrier coatings (EBCs) for protection of ceramic matrix composite (CMC) materials in the hottest portions of gas turbines fueled by pure hydrogen or hydrogen blends.

- Generate performance data to inform the use of current EBCs in hydrogen gas turbines.
- Design new EBCs with improved performance needed to enable future high-efficiency hydrogen gas turbines.







By producing performance data of existing EBCs and designing new EBCs with increased durability in hydrogen combustion environments, this project will help to commercialize high-efficiency hydrogen gas turbines.

Team: R. Oleksak, Ö. Doğan, M. Gao, S. Hao, C. Carney

Developing Capabilities for EBC Testing

Milestone: Design and build a test rig to enable EBC testing in simulated hydrogen combustion environments. **Effort Ongoing**

Simulating gas turbine environments is challenging:

- Ultrahigh temperature (1500 °C +)
- Complex gas mixtures
- Elevated pressure
- High gas velocities
- Thermal cycling

This laser-based heating rig will closely simulate gas turbine environments to enable performance evaluation of existing and newly designed coatings.

Milestone: Establish a partnership to deposit EBCs using air plasma spray methods. **Complete**

• A partnership has been established with Praxair Surface Technologies, a leading producer of coating equipment and services.



Computational Design of New EBCs

Approach: Utilize DFT calculations with combinatorial chemistry methodology to design new EBC systems

Initial Focus: Rare earth disilicate system





Computational Design of New EBCs

Promising new coating compositions identified in the rare earth disilicate system:

- Very good agreement between calculated and experimental CTE and thermal conductivity for current EBC materials such as Yb₂Si₂O₇.
- Calculations enable determining mixed rare earth disilicates with optimal CTE match and ultralow thermal conductivities, without compromising mechanical properties.





Milestone: Design new EBC with enhanced performance using computational approach. **Complete (and ongoing!)**

Future efforts will focus on:

- Experimental validation and performance testing.
- Integrating advanced coating concepts such as selfhealing strategies.
- Strategies to further increase temperature capability (moving beyond Si bond coats).

Design tool for crack-resistant ceramic matrix composites and environmental barrier coatings in hydrogen turbines



<u>Objective</u>: Develop physics-based computational models to predict fracture and crack growth in ceramic matrix composites (CMCs) and environmental barrier coatings (EBCs) and provide guidance for materials design in hydrogen turbines targeting a low-carbon economy.

Program Linkage: Predicting capability of damage and fracture in CMCs and EBCs facilitates public confidence and welfare by supporting safety analyses regarding hydrogen blending, development of materials compatible with hydrogen that ensure the safe use of hydrogen in hydrogen turbines.

Challenge: Physics-based modeling is largely missing for predicting life of CMCs and EBCs due to the complex interactions among various factors. For CMCs, it is required to integrate interfacial sliding, matrix cracking, and fiber breakage in CMCs as well as the effect of thermal cycling and possible phase transformation. For EBCs, it is required to consider crack growth and spallation of EBCs under the influence of thermal cycling and environmental effects.

Our Approach: Develop first-of-its-kind models for fracture and cracking of CMCs and EBCs in hydrogen turbines incorporating *explicitly* the effects of materials microstructure and operating conditions.

Outcome: Computational tools for CMCs and EBCs microstructure optimization for hydrogen turbines.



Creep & Fatigue Modeling

Cheng et al. *Int J. Plast*. (2019) Xue et al. *npj Comput. Mater*. (2022) Xue et al. *IJHE* (2023)

Current State and Market Penetration of CMCs in Utility Gas Turbines and Future Hydrogen Turbines

EY23 Study

- Investigate the current state of EBC/CMC component systems in utility gas turbines and future hydrogen turbines
- This activity shall look at both research and actual applications
- The effort will identify the current pros and cons and options within the industry of this technology for use in utility turbines
- Investigate the likelihood of market penetration of CMCs in utility gas turbines and future hydrogen turbines, including the technical barriers to market penetration
- Ultimately, is this a reached effort NETL should continue to pursue, and if so, what areas should NETL be researching?









Hydrogen Effects on Materials for Hydrogen Production and Utilization

Addressing High-Temperature Hydrogen Attack (HTHA) on Steels Used in Hydrogen Production

Objective and motivation

- To address a critical materials challenge in high-temperature hydrogen production from hydrocarbon fuels high temperature hydrogen attack (HTHA) of structural steels, alloys, and their weldments.
- The ultimate goal of this project is to improve the infrastructural integrity and efficiency of pressure vessels and steam components, and promote hydrogen as a versatile, sustainable, clean fuel.

Task description

- Fundamental understanding of HTHA mechanism of various steels
- Developing integrated testing and modeling tools for optimizing the current HTHA guideline (API RP 941 Nelson curves)
- Designing next-generation HTHA-resistant alloys.

Accomplishment

• The NETL team produced a range of commercially available steel used in the field after consulting with industrial partners, applied different heat treatments to improve their properties, and began studying their mechanical performance.

Future plan

- Finish building the capability of high temperature hydrogen testing facilities at NETL.
- Continue material performance assessment of existing steels.
- Obtain in-service materials from industrial partners and evaluate their performance.



Tesoro Anacortes refinery incident, catastrophic rupture of heat exchanger on April 2,2010.

How does hydrogen interact with materials at high temperatures?



What is the effect on the material integrity?



API Nelson curve for carbon steels

- What is the performance of the existing materials in high-temperature hydrogen environment?
- Is the existing infrastructure reliable for high temperature hydrogen environment?





• Collaborative work and data sharing between NETL, ORNL and industry

Tasks	Subtasks
Task 1: Fundamentals of HTHA & Experimental Evaluations <mark>(ORNL, NETL)</mark>	Task 1.0: Baseline microstructure and mechanical properties of metals and welds currently considered for HTHA applications
	Task 1.1: Assessing effect of hydrogen on microstructural degradation after high temperature service exposure from ex-service material
	Task 1.2: Mechanical damage evaluation in ex-service material) due to high temperature H ₂ environments
	Task 1.3: HTHA susceptibility testing of similar and dissimilar metal welds
Task 2: Development and Validation of HTHA-Prediction Model <mark>(ORNL lead)</mark>	Task 2.1: HTHA-prediction model development
	Task 2.2: HTHA-prediction model validation
Task 3: New Alloy Design and Testing <mark>(NETL Lead)</mark>	Task 3.1: Chemical composition optimization for HTHA resistance and design of new alloy
	Task 3.2: Lab-scale melt and large-scale component fabrication (~10-20 kg material)
	Task 3.3: HTHA susceptibility evaluation of new alloy and its welds
Task 4: Industry Collaboration and Technology to Market	Technology dissemination for regulatory body approval and industry acceptance of the developed HTHA evaluation methodology and new HTHA-resistance alloy (ORNL, NETL, Industry)
(ORNL/NETL/Industry)	

<u>The team</u>

NETL: Stoichko Antonov, Kaimiao Liu, Ömer Doğan, Martin Detrois, Paul Jablonski, Kyle Rozman **ORNL**: Zhili Feng, Yiyu Wang **Industrial partner**: API

Parent grain analysis for PJ steels

• Exploring various commercially available and in-house designed steel compositions

ositions



Multi-scale characterization of composition-microstructure-property relationships +/- hydrogen to understand the effect of hydrogen on material performance.

Ultimate goals: Initial assessment of the performance of the existing materials in hightemperature hydrogen environment enables the transition from fossil energy to clean hydrogen energy.

Carbide EDS analysis for PJ-2 steel



Mechanical properties of select steels

Surface Reactions Modification to Mitigate Hydrogen Embrittlement of Materials

Objective and motivation

- To address a critical materials challenge of H ingress into and embrittlement of structural steels and alloys and a framework to incorporate surface reactions into alloy design, thus enable design of alloys that inhibit H ingress and improve H embrittlement resistance.
- The ultimate goal is to enable development of materials that will ensure infrastructural stability and efficiency of components in the hydrogen economy.

Task description and goals

- Develop fundamental understanding of the material surface chemistry (nominal or of native oxide) on the absorption/adsorption rates of hydrogen into the material, focusing on Fe-based steels
- Develop multi-scale physics-based engineering models to predict and assess hydrogen ingress into a material as a function of its composition, oxide layer, microstructure and other external factors
- Designing next-generation HTHA-resistant alloys, with surfaces optimized for inhibiting hydrogen permeation.

The team

NETL: Stoichko Antonov, Wissam A. Saidi, Richard Oleksak, Lucas Teeter

Material's interaction with hydrogen





- Hydrogen adsorbs to the metal surface
- Can be recombined into H₂ gas (not embrittling)
- Or absorbed into material (embrittling)

How do we prevent hydrogen absorption and promote H₂ gas formation?

Ultimate goal: Develop materials and alloy design tools that enable the transition from fossil energy to clean hydrogen energy by preventing hydrogen permeation and embrittlement.



Transformational Alloys for Hydrogen Service—Development and Manufacturing

DESCRIPTION

- This tasks focuses on the development of alloys and processes, including scale-up to industrial applications, for materials capable to withstand high-temperature operations (>850°C) and demanding environments, such as hydrogen. The task is divided into 4 subtasks:
 - 23.1: Alloy Design and Development for 850°C-1000°C Capabilities
 - 23.2: Scale-Up for Pre-Production
 - 23.3: Alloys Design and Development for >1000°C Capabilities
 (Not discussed in this presentation. Computational modeling and machine learning is used to predict CTE. Ni-alloy with low CTE are designed for protecting CMCs.)
 - 23.4: Alloy Design and Development for Hydrogen Resistance
- Team:
 - PI: Paul Jablonski, Martin Detrois
 - **Key Personnel:** Stoichko Antonov, Michael Gao, Chang-Yu Hung, Xiaotian Fang, Rui Feng, Kyle Rozman
- This task aligns to HQ goals by developing alloys and processes to enable clean energy goals using advanced power generation applications such as those using hydrogen.



AASC Advanced Alloys Signature Center



This task utilizes the unique capabilities of the AASC including:

- 4 VIM furnaces (10-500 lb. capacity)
- Combination VAR/ESR furnace (440 lb. capacity)
- Vacuum heat treatment furnaces including forced Ar gas fan cooling
- Metals fabrication laboratory (forge, hot/cold rolling, 11 heat treatment/hot working furnaces)



Transformational Alloys for Hydrogen Service—Development and Manufacturing

20

Strain (%)

STD

Q SSA

2000

Q

130% increase creep life

4000

Time (h)

6000

Subtask 23.1: Alloy Design and Development for 850°C-1000°C Capabilities

- Develop cast and wrought, cost competitive, alloys for hydrogen-fueled applications in the 850-1000°C range.
- Use of computational tools for alloy design and experimental validation on 8 kg research scale ingots.

ACCOMPLISHMENTS

- NETL custom Q alloy shows 88%-130% increase in creep life compared to commercial alloy HAYNES[®] 282[®] and significantly improved phase stability with a stable matrix necessary for long term mechanical performance.
- Improved understanding of using C to balance fabricability/performance of other alloys.

PUBLICATIONS

- S. Antonov, K.A. Rozman, P.D. Jablonski, M. Detrois, Mater. Sci. Eng. A, 857 (2022) 144049. <u>https://doi.org/10.1016/j.msea.2022.144049</u>
- S. Antonov, C.-Y. Hung, J.A. Hawk, P.D. Jablonski, M. Detrois, Superalloy 718 and Derivatives 2023, Springer Publishing, Pittsburgh PA (2023). <u>https://doi.org/10.1007/978-3-031-27447-3_10</u>
- C.-Y. Hung, S. Antonov, P.D. Jablonski, M. Detrois, J. Alloys Compd. (2023) 170071. <u>https://doi.org/10.1016/j.jallcom.2023.170071</u>

PATENT

• P.D. Jablonski, M. Detrois, J.A Hawk, NiCrCoMoW age hardenable alloy for creep-resistant high temperature applications, and methods of making, **US Patent Application**, **18/194,447**, Filed March 31, 2023.





Transformational Alloys for Hydrogen Service—Development and Manufacturing

Subtask 23.2: Scale-Up for Pre-Production



- The goal is to optimize industrially relevant melting processes used for advanced alloys in existing and emerging energy systems for manufacturing efficiency and cost control.
- Work ongoing with one of the largest US producer of high temperature alloys: exploring ESR process parameters using our research-scale furnace.

ACCOMPLISHMENTS

- Successfully performed a 6 in to 8 in ESR melt by optimizing melt parameters. Next steps include additional study of slag chemistry and effect of ingot composition. (1)
- Enabled the reduction of hydrogen intake in the ingot during electroslag remelting (ESR) by varying slag heat treatment to remove moisture. **Industrial interest in the findings, more work underway. (2)**

PUBLICATIONS

- M. Detrois, P.D. Jablonski, Proceedings of the Liquid Metal Processing & Casting Conference 2022, Philadelphia, PA, pp. 309-318, 2022. <u>https://www.osti.gov/biblio/1889711</u>
- P.D. Jablonski, M. Detrois, Proceedings of the Liquid Metal Processing & Casting Conference 2022, Philadelphia, PA, pp. 203-212, 2022. <u>https://www.osti.gov/biblio/1889721</u>



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Transformational Alloys for Hydrogen Service—Development and Manufacturing



(*)

Subtask 23.4: Alloy Design and Development for Hydrogen Resistance

- Goal: Develop alloys with a unique combination of strength and resistance to hydrogen embrittlement.
- Application temperatures are less than 300°C.
- Approach: Introduce interfaces that tend not to be embrittled by hydrogen and inducing chemical modulations that slow down the hydrogen diffusion, thus reducing the effective hydrogen diffusion rate and increasing strength simultaneously.



- ▲ Formation of deformation twins in low stacking fault energy alloy.
- Stacking faults (SF) in **NETL alloy DT2. Stacking** fault energy was designed to favor fault and twin formation.



Annealed

15% + HT 30% + HT

60% + HT 30% + HT (x2)

ACCOMPLISHMENTS

- A multi-step approach was used to introduce defects which, along with chemical modulations, can slow down hydrogen diffusion.
- The strength of the alloys was significantly increased. In alloy DT2, the ultimate tensile strength increased from 830 to >1200 MPa. (*)

Obtaining Hydrogen-Resistant Superalloys with Wire-Arc Additive Manufacturing



Objective(s)

Develop strategies to improve near-net shape processing and hydrogen resistance for select Ni-based superalloys fabricated by WAAM and other direct energy deposition wire-based additive manufacturing techniques

- Target key commercial solid-solution and precipitation strengthened Ni-based superalloys
- Improve hydrogen resistance by novel processing, heat treatment and/or feedstock modifications
- Expand alloy processing capabilities to include pilot scale wire-drawing

Motivation

Better processing: Improve microstructure and obtain fewer defects in medium-sized components and for repair **Reduce costs for adoption:** Eliminate costly HIP heat treatment through pore-free interlayers and 99%+ dense builds **Hydrogen-compatibility**: Improve understanding of materials issues unique to hydrogen and its impact on performance

Expected Outcomes: (1) Establish baseline properties for WAAM superalloys; (2) Facilitate cost-effective manufacturing & repair with reduced lead times, improved supply chain reliability, added geometric flexibility; (3) Demonstrate path(s) forward to obtain improved hydrogen-resistance for advanced energy system components under hydrogen service

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Laser-wire DED process optimization of Haynes 282

Meltio 450 LW-DED system at OSU-ATAMI

High-power, multi-laser head with small heat affected zones for more controlled wire deposition and potential cost saving to L-PBF AM

Approach: 1) *Single line tracks* to identify rough processing window; 2) *Multiline tracks* for bead geometry & inter-track offset; 3) *Cubes* for process optimization and performance screening after commercial heat treatment

EY22 Milestone - Complete data collection for LW-DED Haynes 282 process optimization (3/30/23)

Key outcomes:

- Hands-on operation of the Meltio 450 LW-DED system
- Varied travel speed, laser power, & inter-track off-set & determined microstructural relationships (porosity, fine grain colonies, etc.)
- 99.9%+ density achieved for a range of conditions
- Comparable yield strength of 715 MPa to conventional Haynes 282
- Small deviations in yield strength with processing conditions correlated to the aggregate grain size (Hall-Petch)

Next steps:

- Finish microstructure screening & compression testing at 750°C
- Publish soon the results of LW-DED 282 process optimization study

Conference presentations: 1) K. Tippey and C.K. Sudbrack , TMS 2022; 2) R. Feng, K. Tippey and C.K. Sudbrack, TMS 2023



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Evaluation of WAAM Haynes 282

Gefertec Arc 605 WAAM system with U. Pittsburgh

Leverage outcomes from 2-year UCFER project on location specific design of WAAM 282 with high-throughput experiments & machine learning

- Solution temperature identified for grain recrystallization
- Custom aging conditions identified for improved properties
- NETL-RIC: Technical monitor and collaboration with limited tensile/creep

Fronius Cold Metal Transfer (CMT) TimedTwin GMAW

Advantages: 1) Low spatter dip arc process; (2) Ultra-low heat input transfer for small heat affected zone; (3) Low dilution of base metal; (4) Fast deposition up to 30 kg/h

Contract for deposition trials in place March 2023 after delays

Next steps:

- Build a robust research execution plan collaboratively with ORNL
- Process optimization of WAAM Haynes 282 with Oregon State using single track and simple multi-track builds
- Demonstrate simple wall builds for characterization & preliminary baseline property evaluation
- Identify hydrogen mitigation strategies and begin hydrogen resistance screening to inform down selection



Oregon State University Metals Manufacturing Research Group





Physics Based Machine Learning of Alloy Oxidation Performance

OBJECTIVES

- Predict conditions (e.g. alloying compositions) for forming protective oxide scale (such as Cr_2O_3 and α -Al₂O₃) for steels, nickel-base superalloys, and FCC-based high entropy alloys
- Predict oxidation rate constants and spallation
- Develop multi-objective machine learning platform to optimize mechanical and environmental properties

APPROACHES

 Integrate data collection and management, multiscale computational modeling design, machine learning approaches, and experimental validation, coupled with an appreciation for the underlying physical processes driving the alloy oxidation reaction

DELIVERABLES

• Design cost-effective alloys with superior oxidation resistance to the current-state-of-the-art commercial alloys for hydrogen turbine hot path





A. Ross et al. Tailoring critical Al concentration to form external Al2O3 scale on Ni–Al alloys by computational approach. Journal of the American Ceramic Society. 2022;105:7770-7

TEAM

- PI: Michael Gao
- Co-PI: Richard Oleksak, Madison Wenzlick
- Key Personnel: TBD, William Trehern

ALIGNING TO HQ GOALS

 Developing predictive tools for accelerated design of cost-effective hightemperature alloys with superior oxidation resistance for hydrogen combustion applications achieving net-zero GHG emissions by 2050. 23





O. Mamun et al. Machine learning augmented predictive and generative model for rupture life in ferritic and austenitic steels, Npj Mater. Degradation 5(1) (2021).

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- <u>Task 20</u> Design and Evaluation of Environmental Barrier Coatings for Protection of Ceramic Matrix Composites in Hydrogen-Based Turbines
- <u>Task 21</u> High-Temperature Hydrogen Attack on Steels Used in Hydrogen Production
- <u>Task 22</u> Obtaining Hydrogen-Resistant Superalloys with Wire-Arc Additive Manufacturing
- <u>Task 23</u> Transformational Alloys for Hydrogen Service Development and Manufacturing
- <u>Task 24</u> Design tool for crack-resistant ceramic matrix composites and environmental barrier coatings in hydrogen turbines
- <u>Task 25</u> Physics Based Machine Learning of Alloy Oxidation Performance
- <u>Task 26</u> Current State and Market Penetration of CMCs in Utility Gas Turbines and Future Hydrogen Turbines
- <u>Task 27</u> Surface Reactions Modification to Mitigate Hydrogen Embrittlement of Materials

Advanced Materials Development for Hydrogen Production and Energy Systems

VISIT US AT: www.NETL.DOE.gov



@NationalEnergyTechnologyLaboratory

CONTACT: Ömer Doğan, Technical Portfolio Lead omer.dogan@netl.doe.gov

