Multiscale Modeling of Corrosion and Oxidation Performance and Their Impact on High-temperature Fatigue of Automotive Exhaust Manifold Components

Project ID: MAT163

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Overview

Timeline

- Project start date: November 2018
- Project end date: October 2021
- Percent complete: 15%

Partners

- The Ohio State University
- Missouri Science and Technology
- Oak Ridge National Laboratory

Budget

- Total project funding
  - DOE share: $2.0M
  - Contractor share: $0.58M

Barriers

- Micro- and meso-scale corrosion and oxidation performance models
- Corrosion/oxidation-fatigue model
- Experimental validation of performance Model
- Component level demonstration

Project Objectives

- To develop multiscale computational models capable of predicting the location and extent of high-temperature corrosion/oxidation of automotive exhaust manifold materials (cast steels, Ni-resist and cast iron) for temperature up to 1050^{o}C.
- To conduct static and thermal cycling corrosion/oxidation trials in controlled atmosphere, and demonstrate the model capable of predicting the corrosion/oxidation performance to within 10% of experimental measurements.
- To develop a robust computational model to predict the high-temperature fatigue life of the material under corrosive/oxidizing conditions, and demonstrate the model capable of predicting the corrosion/oxidation-fatigue performance to within 10% of experimental measurements.
- To demonstrate the predictive utility of the developed corrosion/oxidation-fatigue model in accelerating the development of new exhaust manifold alloys.

Tasks and Budget Period

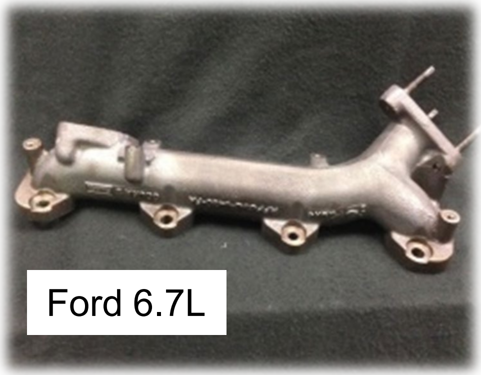
Tasks	BP1: SiMo-type Cast Iron				BP2: Cr20Ni10-type Cast Austenitic Steel				BP3: Model Demonstration on Components			
	1	2	3	4	5	6	7	8	9	10	11	12
Task 1: Project Management and Planning												
1.1 Update Project Management Plan												
1.2 Project Management												
Task 2: Development of Corrosion/Oxidation Performance Model					A				D			
2.1 Density Functional Theory Calculation												
2.2 Higher Length Scale Simulation from MD, KMC, and PEL												G
2.3 Development of Modified Wagner Kinetics Model												
Task 3: Experimental Validation of Corrosion/Oxidation Performance Model					B				E			
3.1 Isothermal Corrosion/Oxidation Trials in Controlled Gas and Characterization Trough XPS, SEM, TEM and Raman Spectroscopy												
3.2 Cyclic-thermal Corrosion/Oxidation Trials in Controlled Gas and Characterization Trough XPS, SEM, TEM and Raman Spectroscopy												
3.3 Isothermal Corrosion/Oxidation Trials in ACEC Gas and Characterization Trough XPS, SEM, TEM and Raman Spectroscopy												
3.4 Cyclic-thermal Corrosion/Oxidation Trials in ACEC Gas and Characterization Trough XPS, SEM, TEM and Raman Spectroscopy												H
Task 4: Development of Corrosion/Oxidation-Fatigue Model					C				F			
4.1 TMF Testing on Ex-situ Corroded/Oxidized Samples												
4.2 TMF Testing on In-situ Corroded/Oxidized Samples												I
4.3 Development of Corrosion/Oxidation-Fatigue Model												
Task 5: Validation and Demonstration of Corrosion/Oxidation-Fatigue Model												J
5.1 Validation of Corrosion/Oxidation-Fatigue Model												
5.2 Demonstration on 6.7L Diesel Cylinder Head Exhaust Manifold Component												K
5.3 Demonstration of the Acceleration of New Materials Solutions												

Background

Exhaust manifold

Collects and routes the exhaust gas produced by the engine to the rest of the exhaust pipe system.

- **Mid-1990's switched from cast iron to HiSiMo cast iron**
  - Oxidation resistance, Si/Mo, higher temperature applications (~850°C metal temperature)
- **Stainless Steel - higher temperature applications**
  - Oxidation resistance, Cr/Ni (~950°C metal temperature)
- **Current/Future -** increase fuel economy and reduce pollutant emissions
  - EcoBoost >1000°C exhaust temperatures



Background

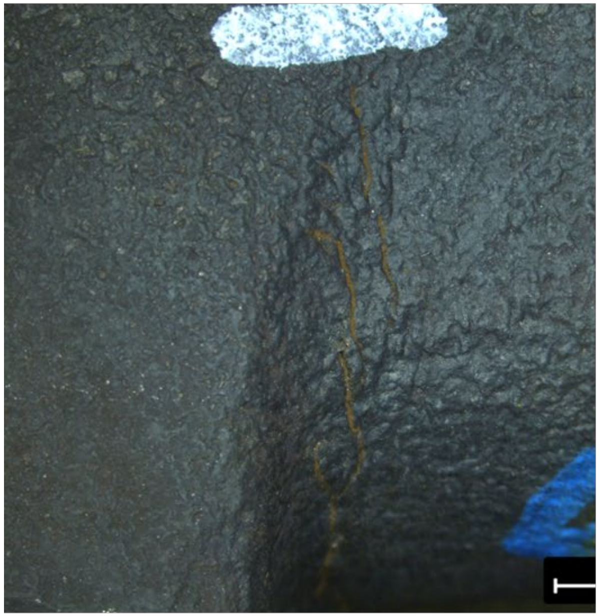
Vehicle Test

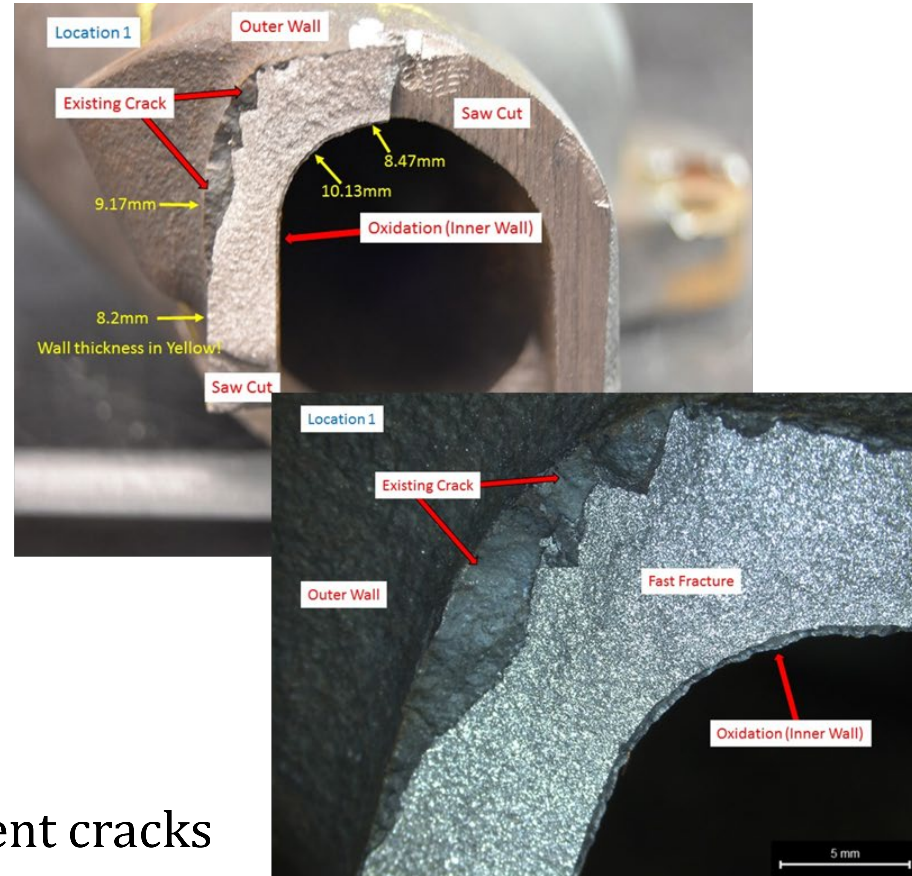
Observation

- Oxidation/Corrosion Layers on fracture surface

Background

Dyno Test Exhaust Manifold





Observation

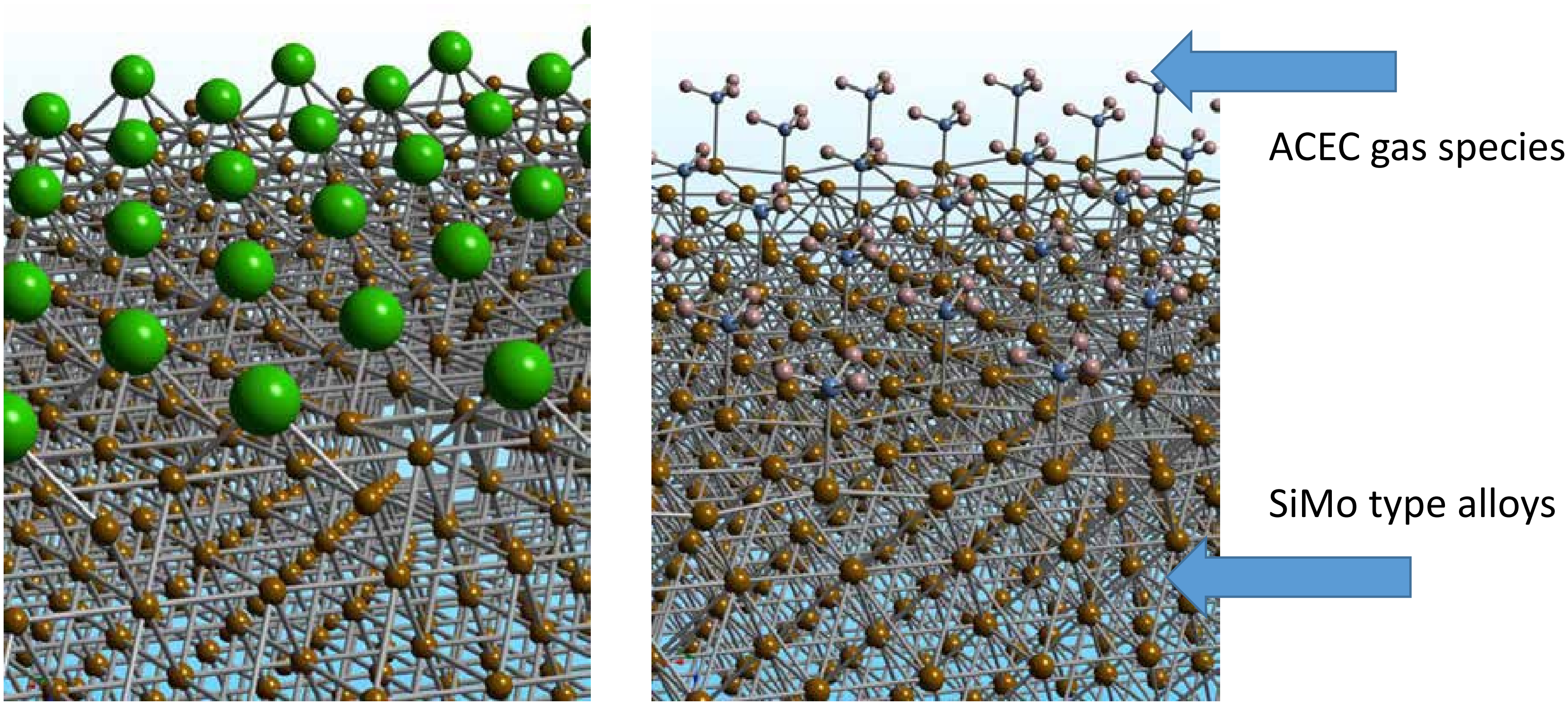
- Outer Surface - Many independent cracks
- Uniform oxidation along inner surface
- Crack occurred near compound radius

Corrosion/Oxidation TMF Modeling Approach

- Assess the fundamental mechanisms of corrosion and oxidation performance of exhaust manifold components in dry and wet air, as well as ACEC gas environment
- Develop atomic level models through integration of advanced computational technologies, including Density Functional Theory (DFT), Reactive Force Field Molecular Dynamic (ReaFF MD), kinetic Monte Carlo (KMC), and Potential Energy Landscaping (PEL)
- The microstructure level Wagner kinetics model will be built upon the results from atomic level modeling
- Develop a phenomenological corrosion/oxidation-fatigue model based on the multiscale corrosion/oxidation model developed in this program, the extensive high-temperature durability database, and thermomechanical fatigue (TMF) model

Corrosion/Oxidation Performance Model

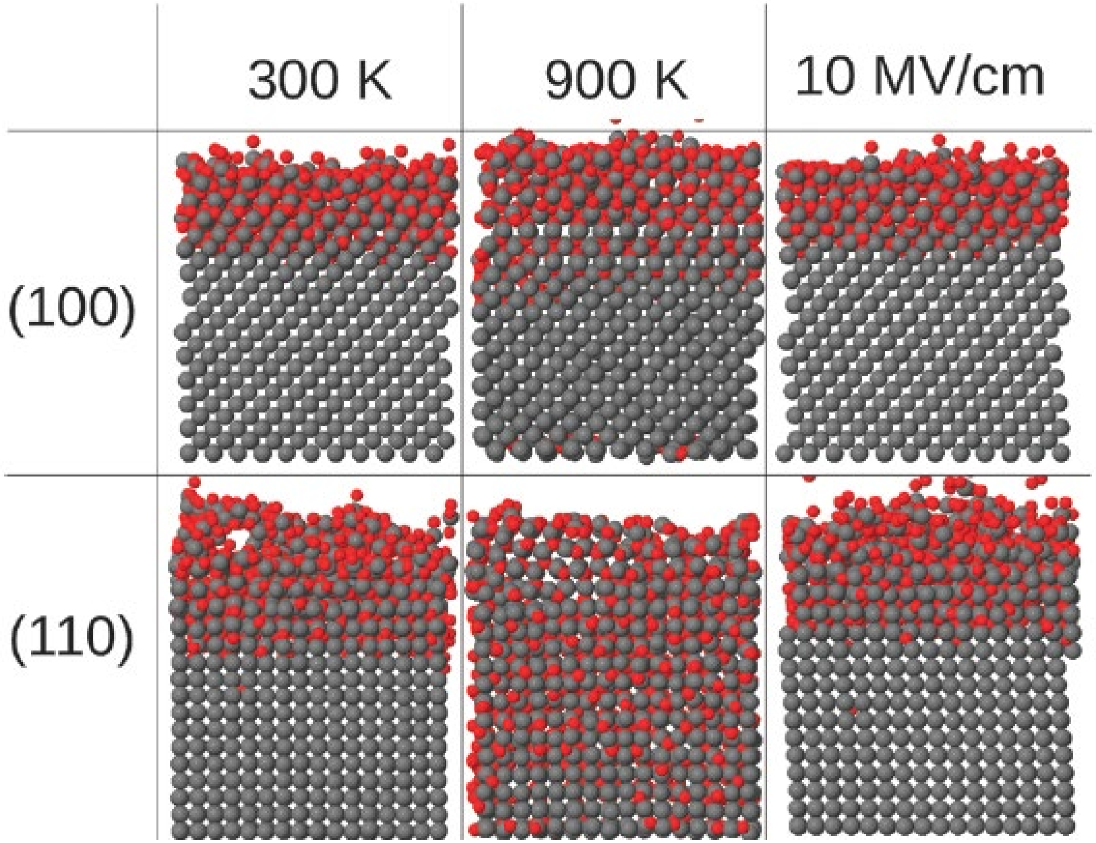
- Density Function Theory (DFT) calculation of the absorption energy for SiMo type alloys (ferrite) with ACEC gas species, dry air or water vapor



C. D. Taylor, Corrosion **68**, 591 (2012).

Corrosion/Oxidation Performance Model

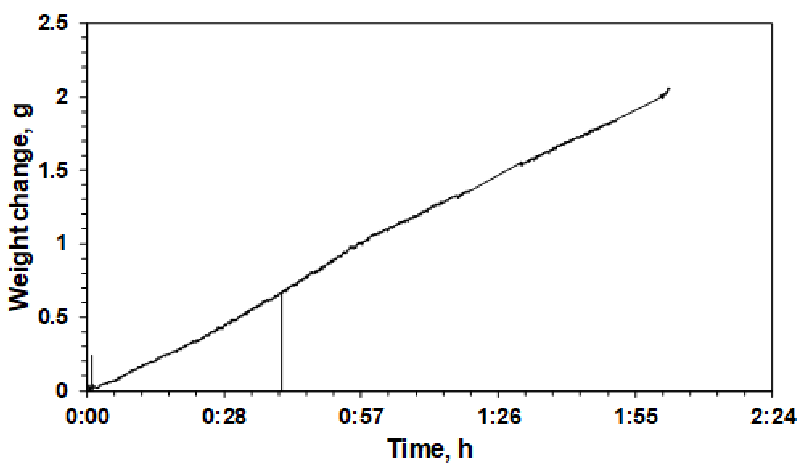
- Reaction Force Field Molecular Dynamic (ReaxFF MD) modeling simulation of the interaction of ACEC gas chemistry with the SiMo type alloys surfaces

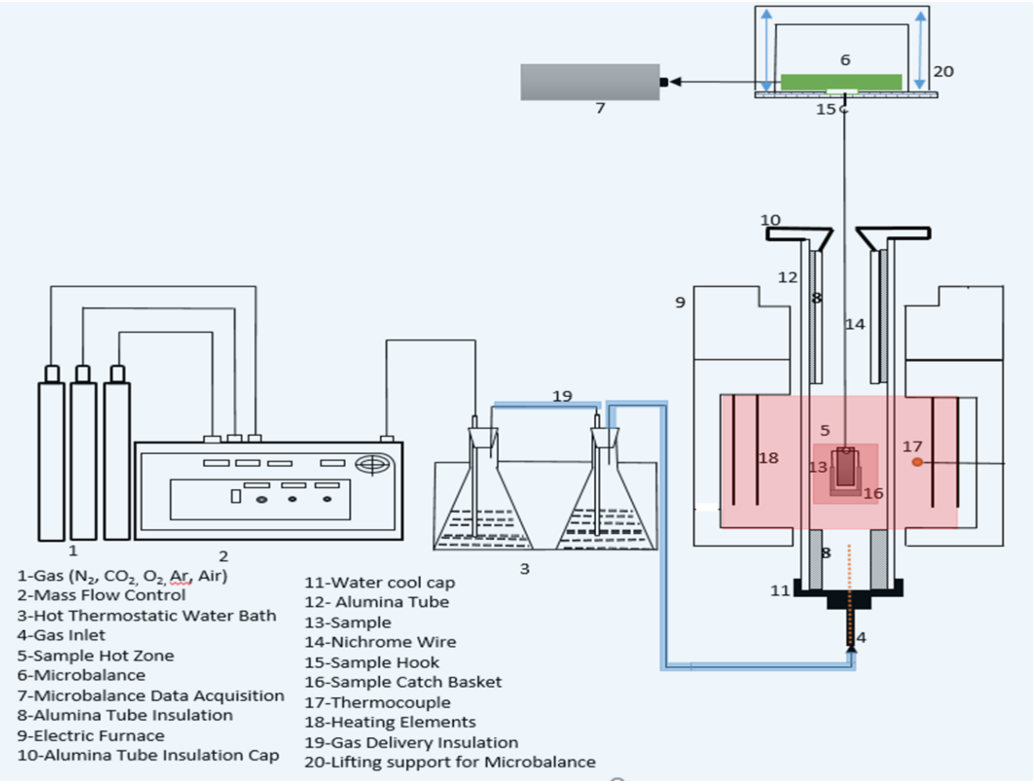


T. P. Senftle, A. C. T. van Duin, et al., npj Computational Materials 2, 1(2016).

Experimental Characterization

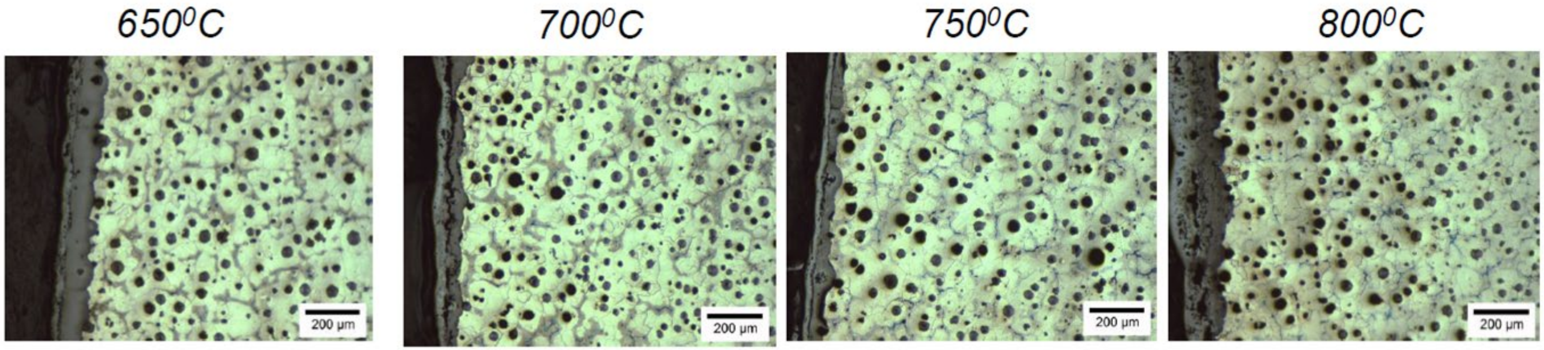
- Several experimental methods, such as X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), and high-resolution Raman spectroscopy, are employed to validate the multiscale computational model at different length scale
- Static and cyclic oxidation kinetics in controlled environment are characterized

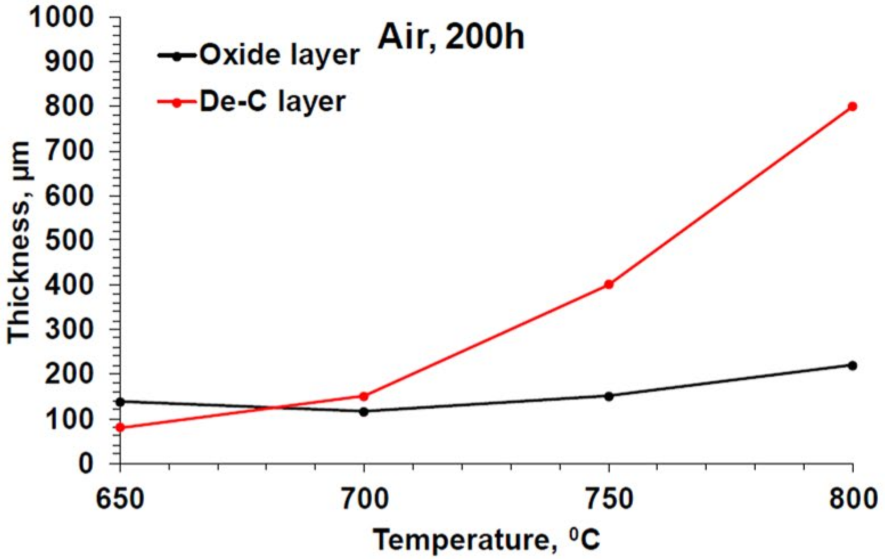




Experimental Characterization

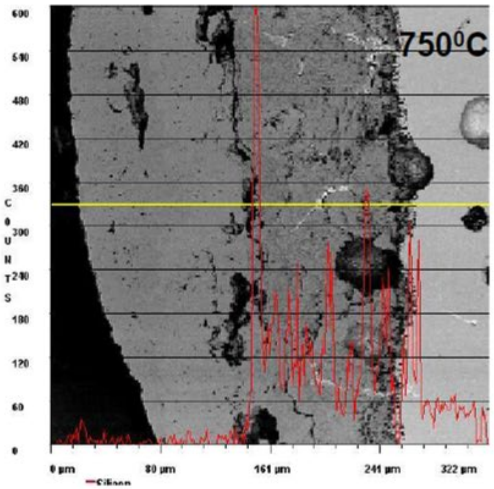
- **Metallography in cross section**
  - Base SiMo alloys in air

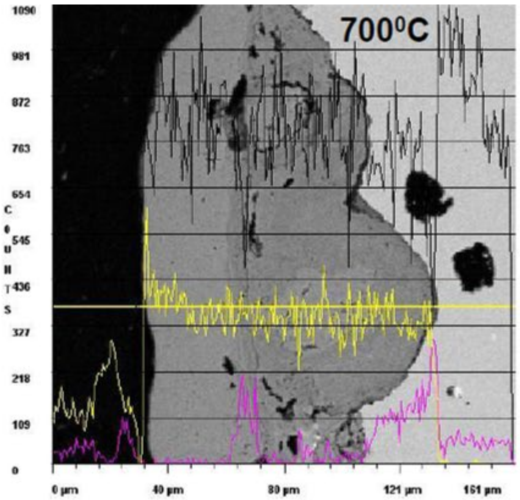


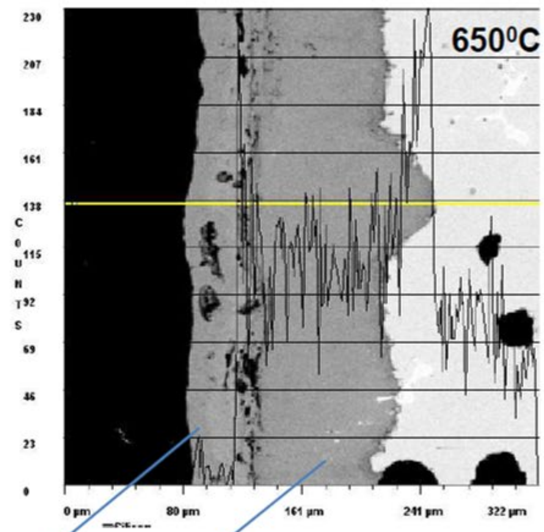


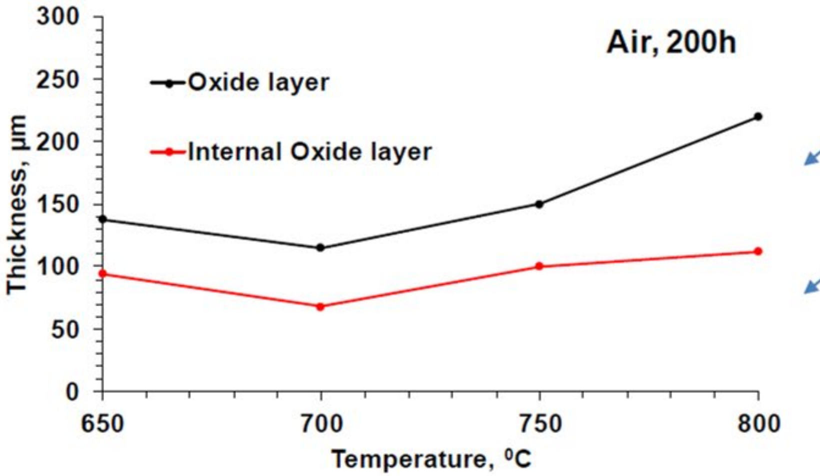
Experimental Characterization

- **Chemistry of Oxidized Surface - Base SiMo alloys in air**



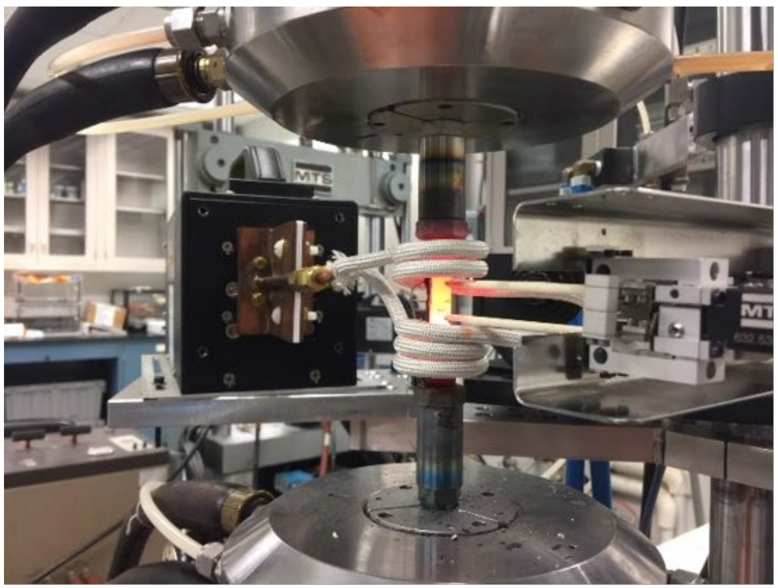


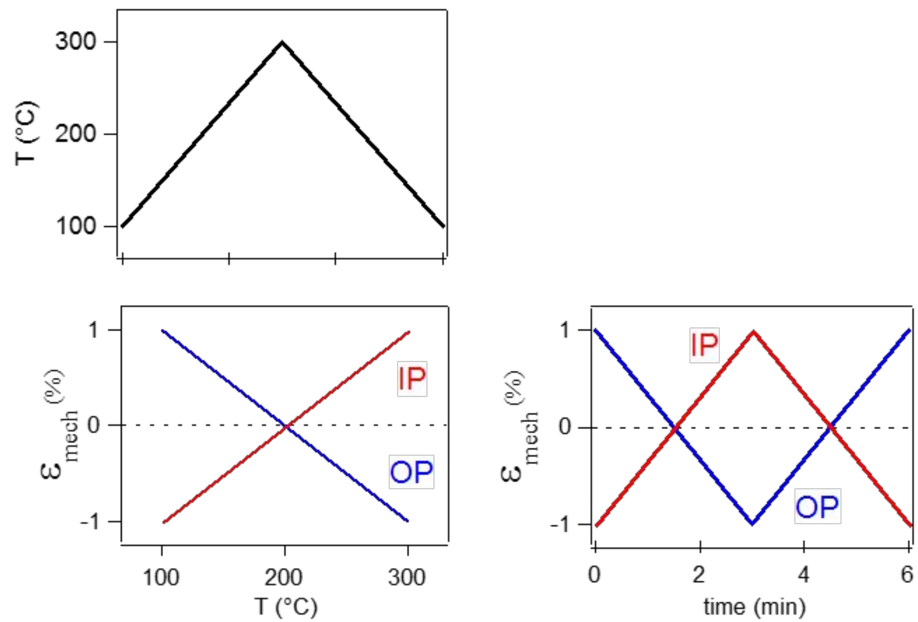




Experimental Validation

- Thermal cycling induces stresses causing elastic or plastic deformation of the oxide scale, as well as oxide spallation, leading to further oxidation of the alloy and fracture into the turbocharger
- Validate the phenomenological corrosion/oxidation-fatigue model





Summary of Budget Period 1 (BP1)

Theoretical modeling and experimental validation of corrosion/oxidation performance and corrosion/oxidation-fatigue of SiMo-type cast iron

- Develop multiscale models for the corrosion/oxidation performance of cast iron alloys (bcc-Fe with alloying elements of interest) using advanced computational methods
- Characterize the corrosion/oxidation performance in terms of nodularity and microsegregation change, grain boundary degradation, as well as oxide film thickness and compositions evolution
- Validate the corrosion/oxidation model to within 10% of experimental measurements
- Conduct TMF tests on both ex-situ and in-situ corroded/oxidized samples in controlled gas environments (inert gas, air, water vapor and exhaust gas)
- Develop and validate a phenomenological corrosion/oxidation-fatigue model for SiMo-type cast iron capable to within 10% of experimental measurements