DNV·GL

ICME for Advanced Manufacturing of Ni Superalloy Heat Exchangers with High Temperature Creep + Oxidation Resistance for Supercritical CO2

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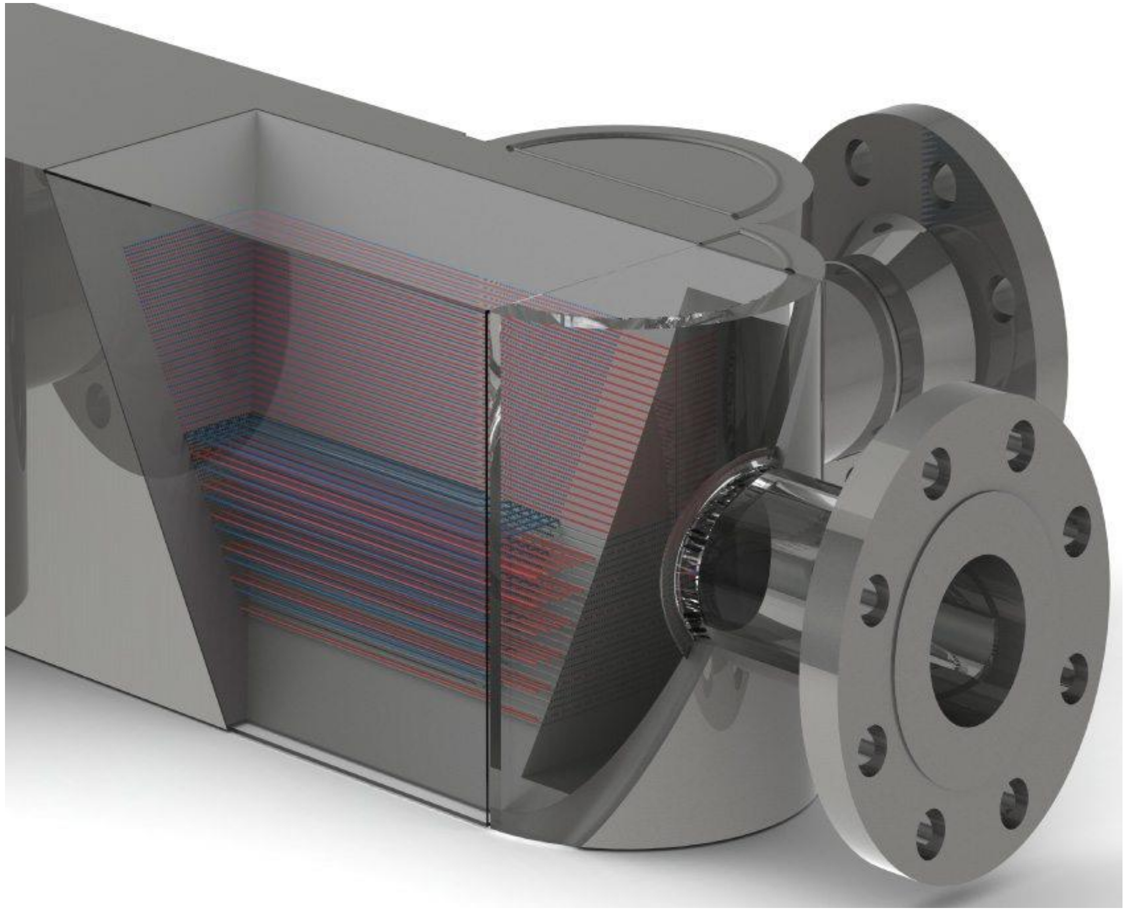
Talk Outline

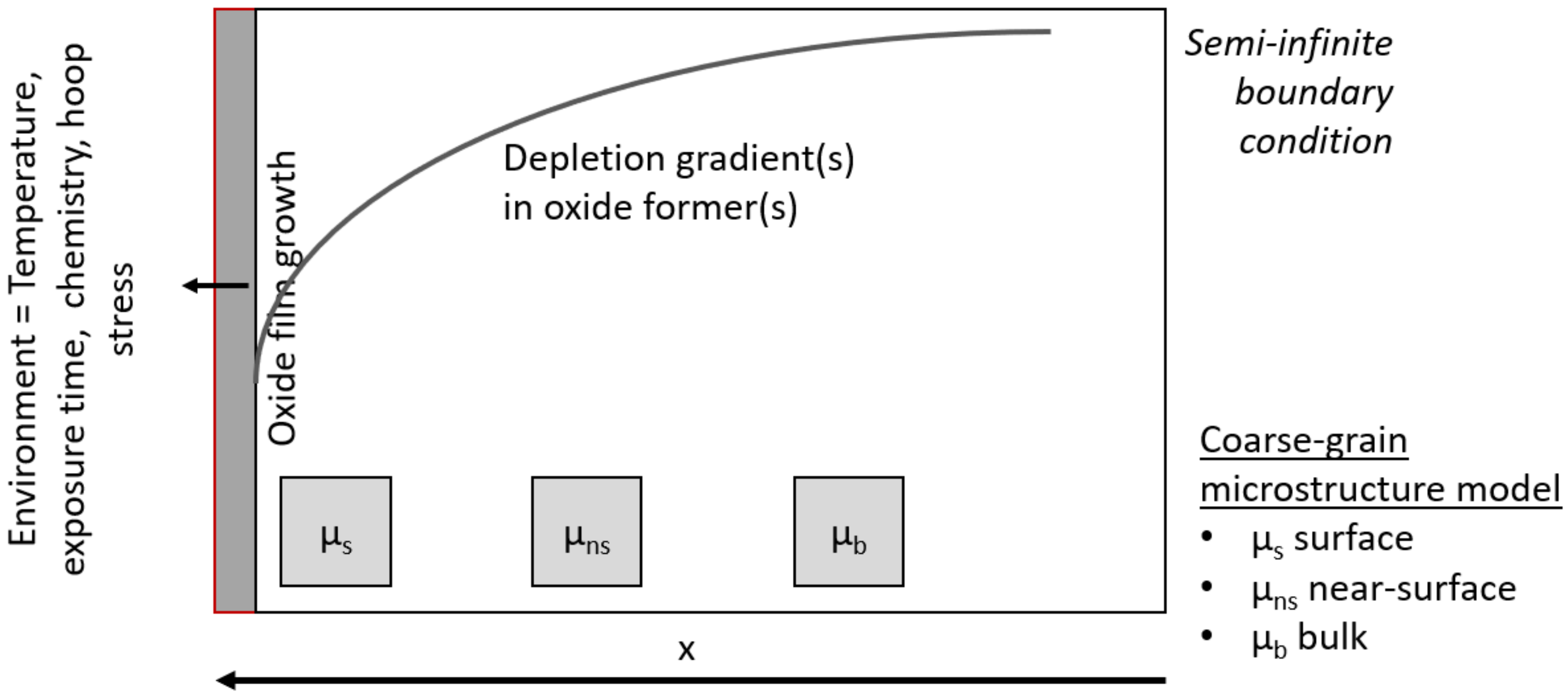
- Objective
- ICME Modeling Tasks
- High Temperature Oxidation Modeling
- Creep Modeling
- Integration with Phase Field
- Advanced Manufacturing of Multi-Material HX Components
- Testing and Characterization
- Milestone Review

Objective

- Microchannel heat-exchangers with optimal durability
- Targeting additive manufacturing design for supercritical CO_2 power
  - 700-1000 C, 50+ years
- Optimized material combinations:
  - Surface skin: alumina former, such as Haynes alloy 224 (high temperature oxidation resistance)
  - Internal layer: chromia former having high creep resistance
- Avoid internal oxidation and dissolution of γ' in near-surface
- Develop and Validate an Integrated Computational Materials Engineering approach to materials design



ICME Strategy



Continuous chemical/microstructure/strength model

d(t) oxide film growth rate from Wagner kinetics

→ C(x,t) from oxidation/diffusion model/DICTRA

→ μ(x,t) from thermodynamics analysis

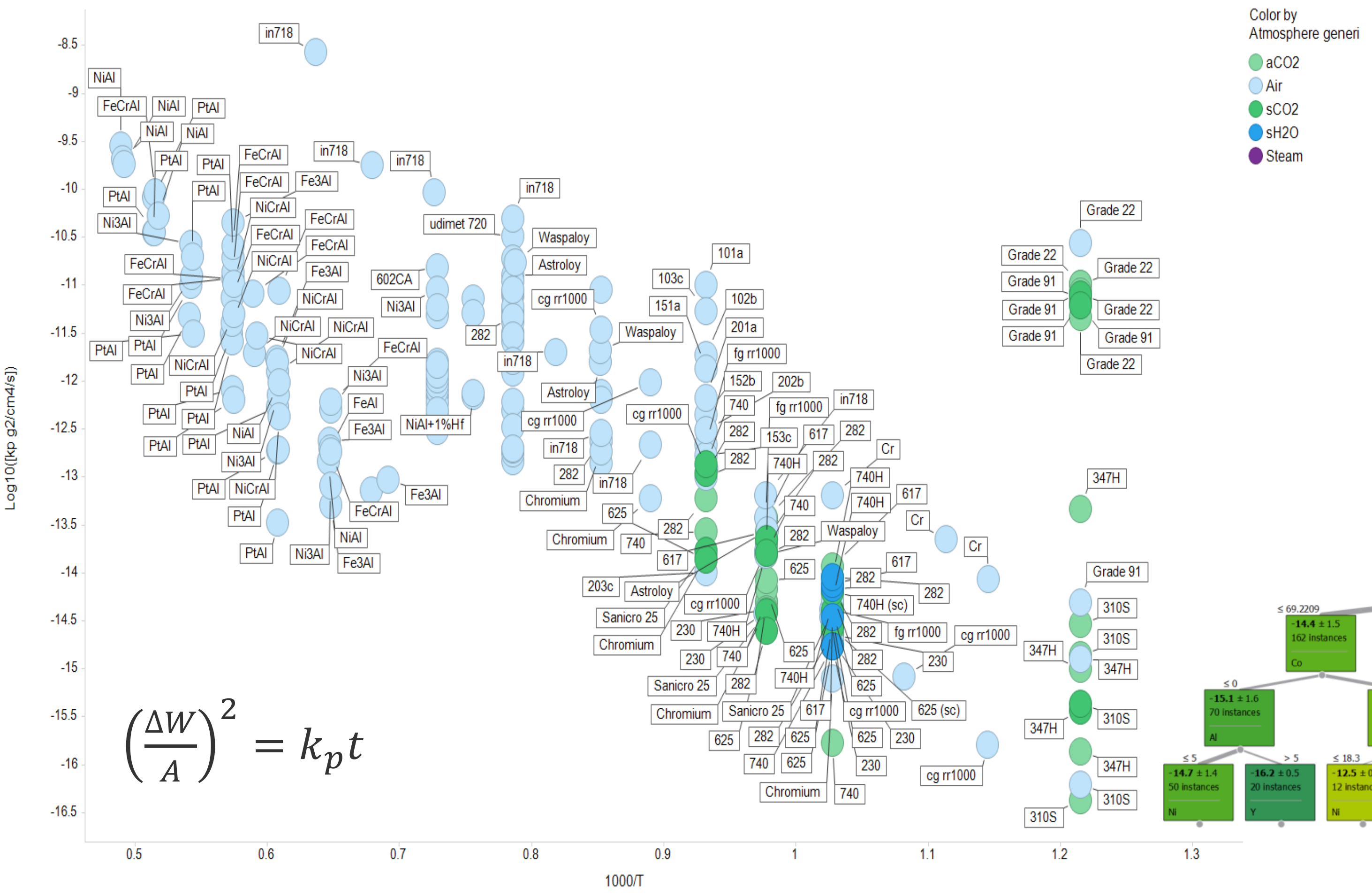
→ S(x,t) from coupled phase field/crystal-plasticity

An integrated model tackling creep-oxidation failure mode of superalloy materials must address:

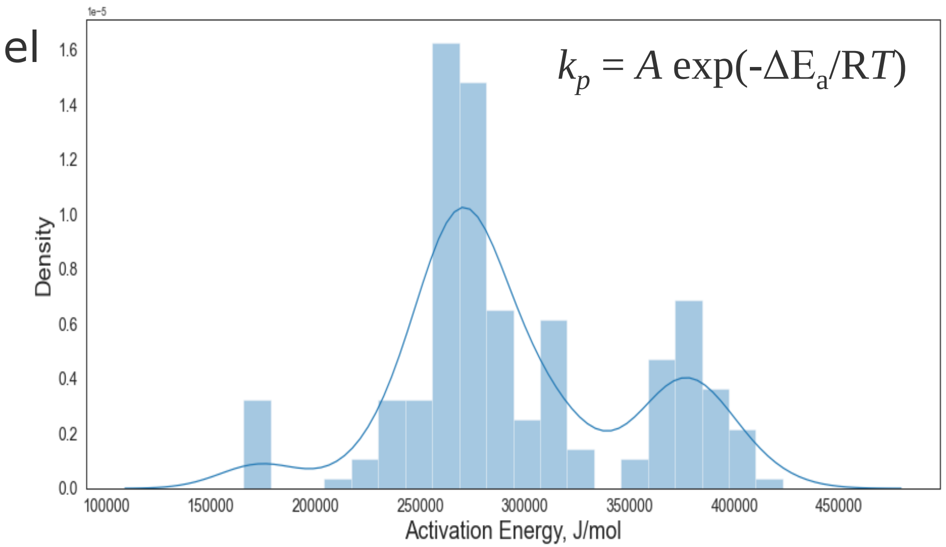
- ❑ Rate of oxidation
- ❑ Rate of materials diffusion
- ❑ Phase transformation
- ❑ Strength evolution
- ❑ Creep dynamics

High Temperature Oxidation Modeling

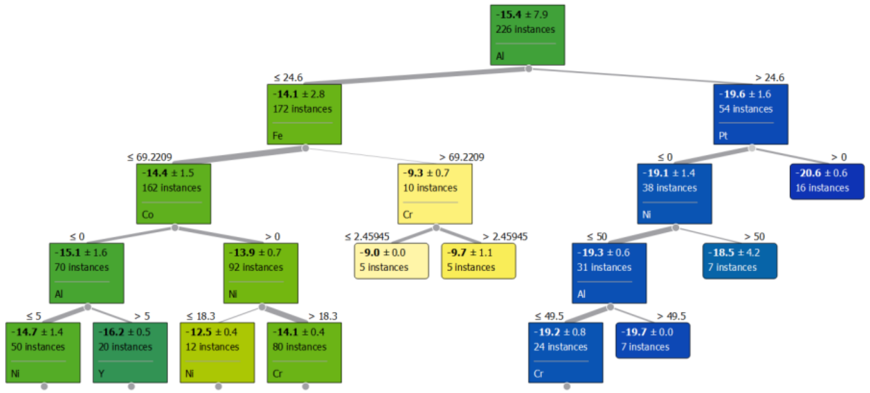
Data curation, analysis and application of a ML-based Arrhenius model



$$\left(\frac{\Delta W}{A}\right)^2 = k_p t$$



$$k_p = A \exp(-\Delta E_a/RT)$$



	MSE
Linear (Ni, Cr, Al)*	1.69
Linear*	0.99
NN	0.81
SVM	1.03
KNN	0.78
Tree	0.82
Random Forest	0.72

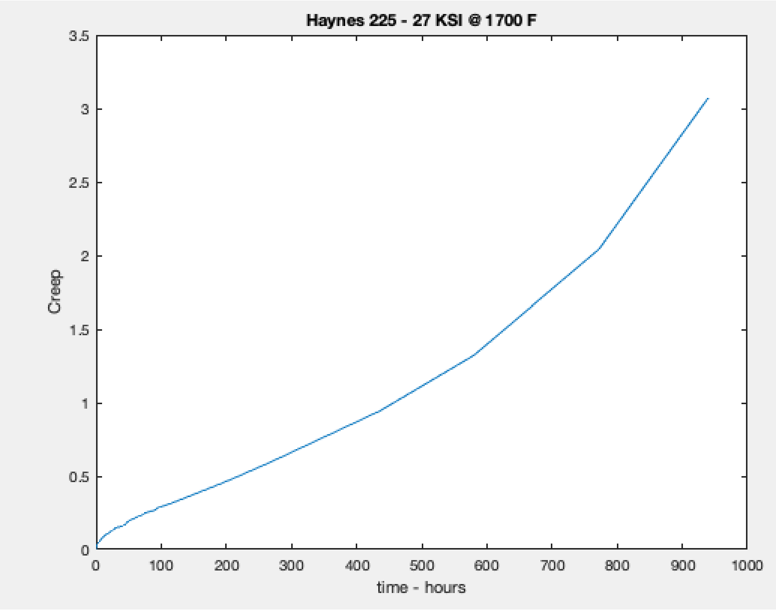
*Manuscript complete and preparing to submit by 9-30-2020

Creep Modeling

- Progress
  - Creep modeling framework developed under NETL Grant No. DE-FE002776 has been adapted for use to predict creep in response to the evolution of γ' structure due to in-service oxidation.
  - Currently undergoing testing
  - Creep data for Haynes 224 (provided by Vinay Deodeshmukh of Hayes International) has been sorted/organized and processed for use to calibrate creep model
  - Calibration of models for Haynes 282 and 224 Underway

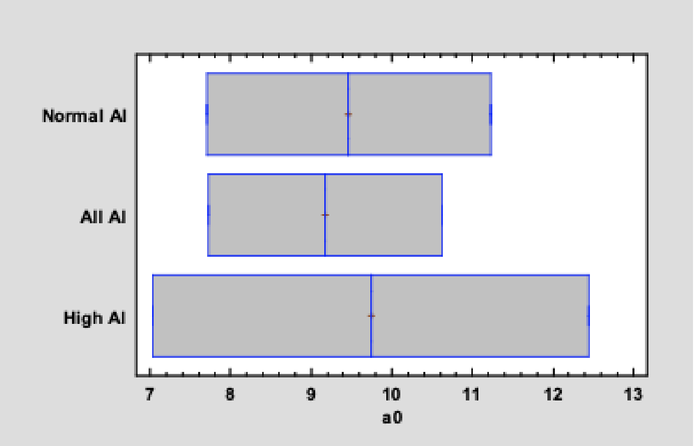
- Upcoming Activities
  - Simulations of oxidized Haynes 282 samples are underway and will be detailed in the next report
  - Preliminary creep simulations on as received Haynes 224 will also be presented.
  - Continued cleanup of test data from Haynes

Raw Creep Curves from Haynes



$$\log(stress) = a_0 + a_1 * LM + a_2 * LM^2$$

$$LM = T_{abs} * [C + \log(hours)]$$



DICTRA Simulation Setup
flux boundary condition with k_p from Chris

$$J_{Al}^{out} = \frac{2k_p}{V_{ox}}\left(\frac{bM_0}{aV_m}\right)(2k_c t + t_0)^{-1/2}$$

At 700℃, k_p=2.3 × 10^{-15} $g^2/cm^4/s$

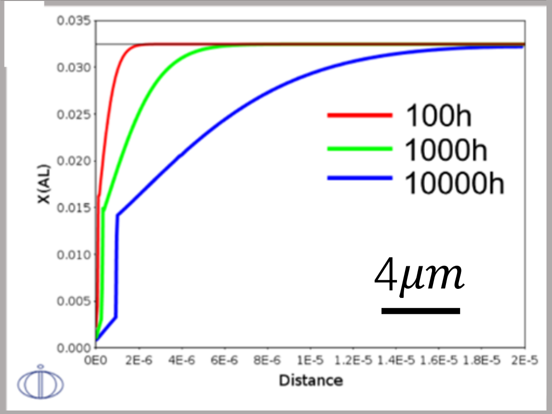
(Pint et al. Mat High Temp 35:39-49 2018)

Al_2O_3 layer

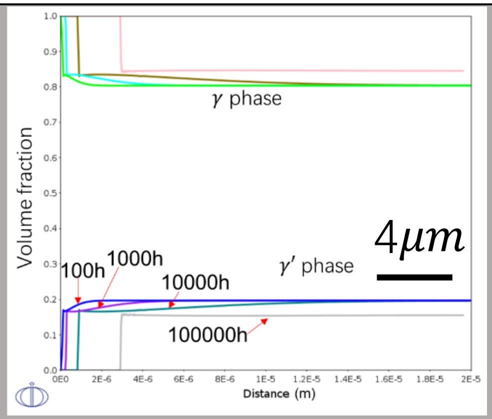
DICTRA calculation

DICTRA Simulation result

Concentration profile



Volume fraction of phases

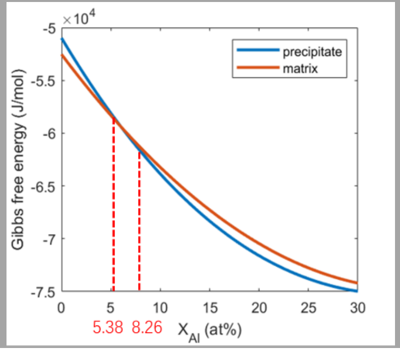


- Precipitates-free zone forms due to the loss of Al.
- Precipitates dissolves up to 3.4% of total volume in the two-phase region

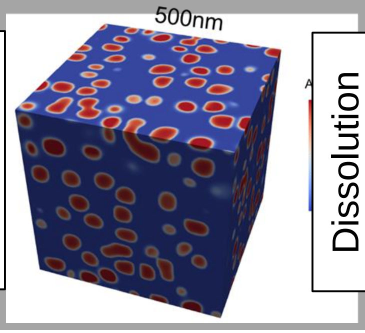
Simulation of particle dissolution and prediction of heterogeneous microstructure: phase field method

ICME approach

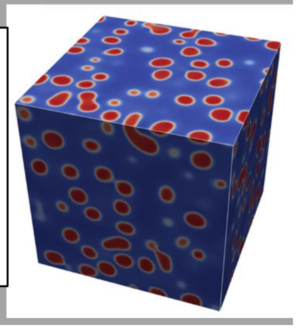
Phase field model (PFM) & results



precipitation



Dissolution

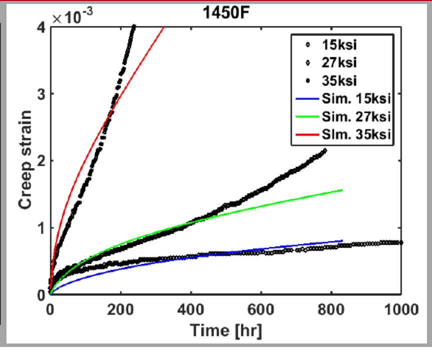


Simulation of creep

Crystal plasticity method

Crystal plasticity model

Homogenized model



Predict the creep behavior with microstructure obtained through PFM

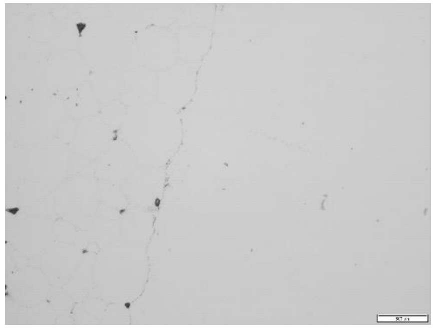
Synthesis of Novel Composition-Gradient Materials

- Weld overlay to mimic the bi-material and collect oxidation and phase-transformation/ageing data

Haynes 282 sheet with 224 weld overlay in place

HIP Cans after HIP by Quintus

Cross section of HIP tubular

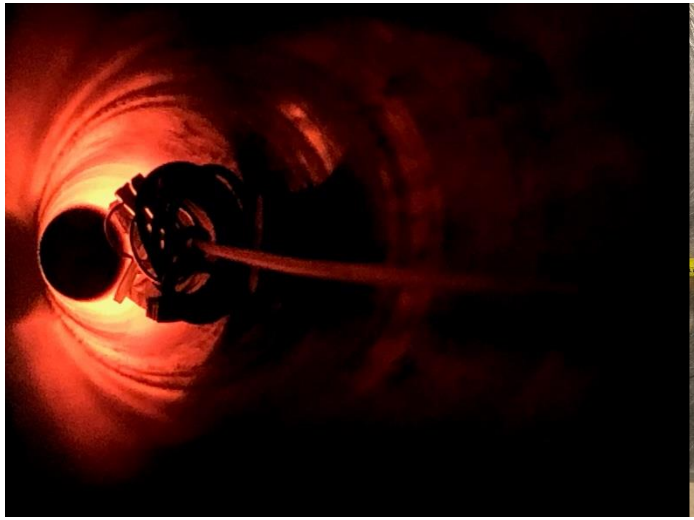


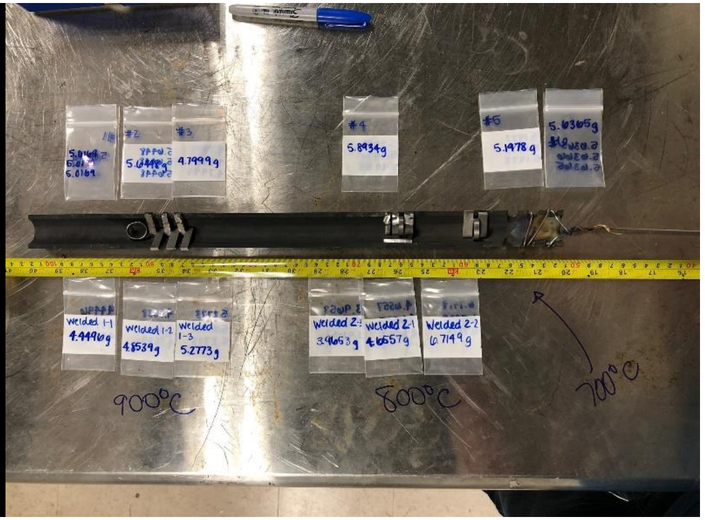
Microscopic image of metallurgical bond region

- Tubular with PM and HIP/HT
  - 224 tubular, packed with 282 powder around a steel core
  - HIP treatment to consolidate and provide metallurgical bond
- Quintus Technologies has provided at no-cost research support in advising on methods and to fabricate tubular samples with HIP
  - Round one: no metallurgical bond was created
  - Round two: good metallurgical bond, samples currently being characterized
  - Next steps: Heat treatment and creep testing

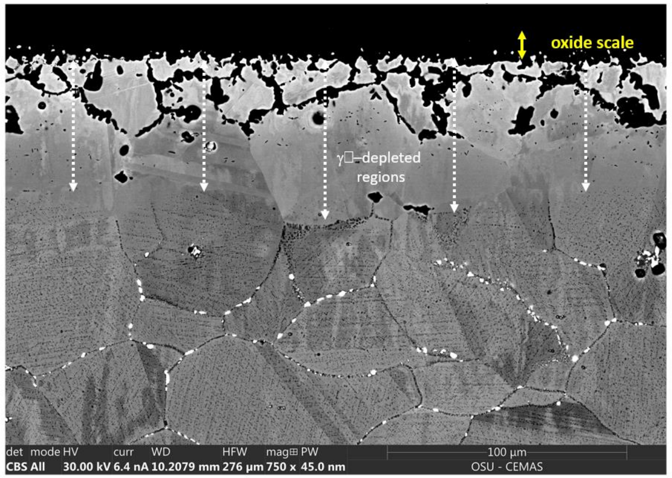
Testing and Characterization

- Exposure tests begun 8/18/2019 at 900C, 800C, and 700C.
  - First interval exposure is 900 hours (10/4/2019)
  - Second interval will be ~5,000 hours (209 days) or March 16, 2020
  - Finally ~10,000 hours (417 days) or October 2020
  - The environment is carbon dioxide at 1 atm.



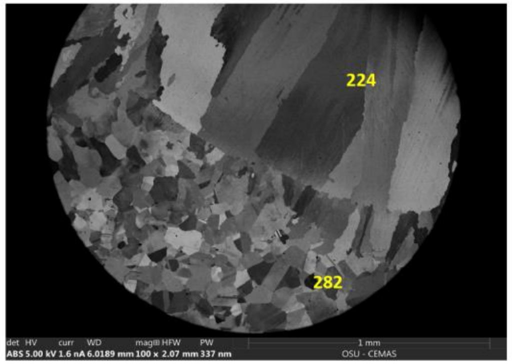


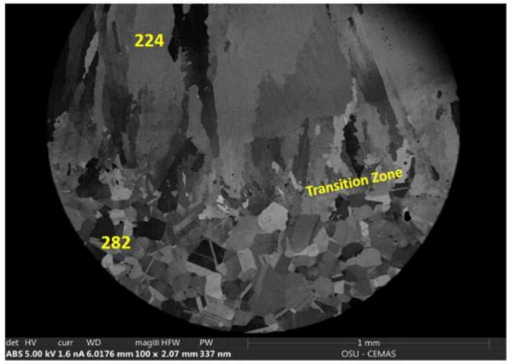
Oxidized and y’ depleted regions visible in SEM



- γ –depleted regions are marked in red lines above.
- The depth of depleted region varies between 55 – 67 µm.

Weld-overlay showing dissimilar grain structure in 224/282

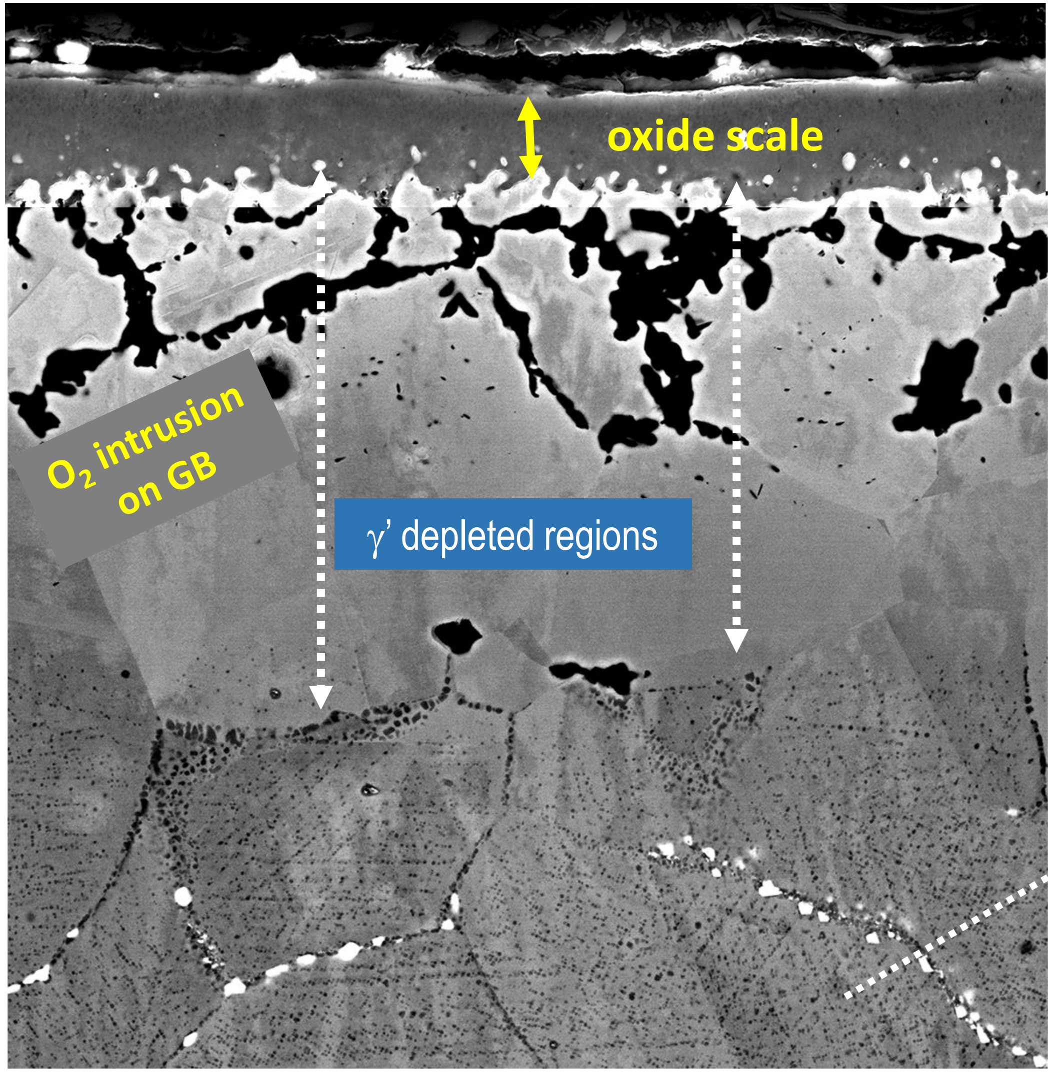


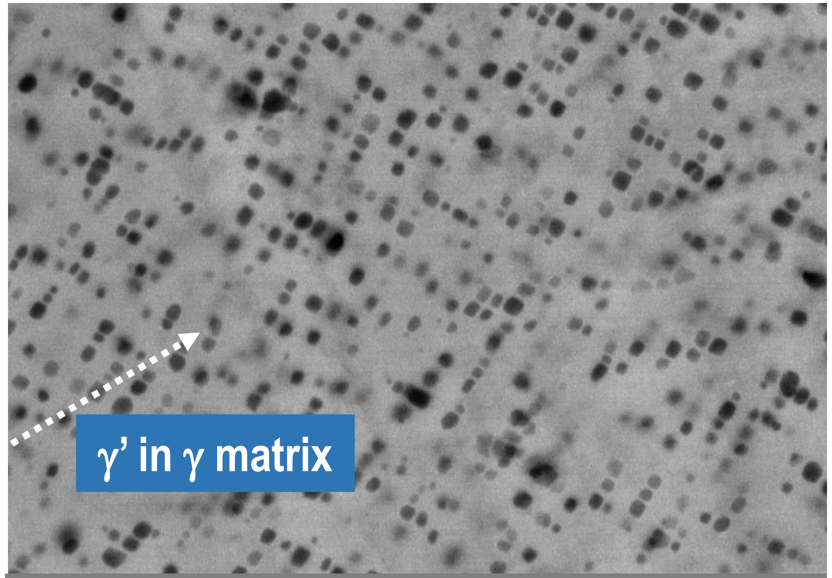


Typical Example of high-resolution Imaging in the SEM to characterize the extent of γ□ precipitate dissolution

Alloy 282- Exposed at 925°C,1000 hrs

The depth of γ’ depleted region varies between 55 – 67 μm.



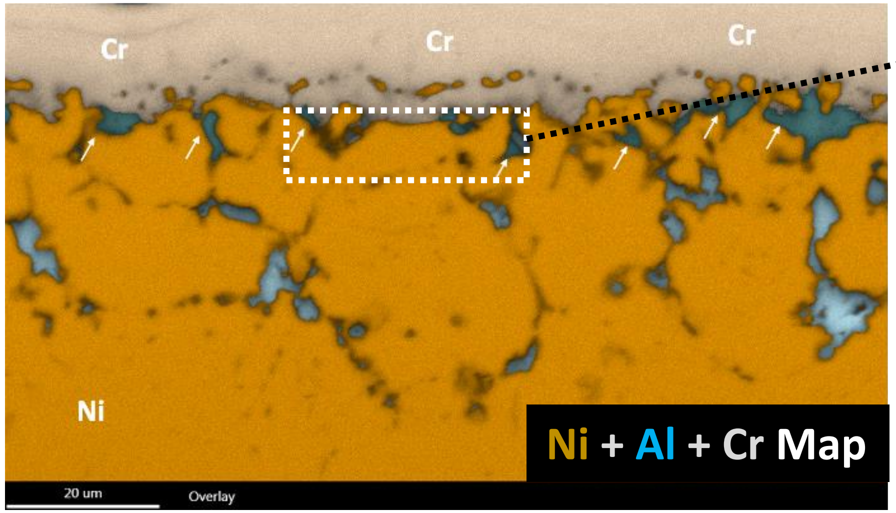


Imaged with Thermo Scientific Apreo FEG-SEM

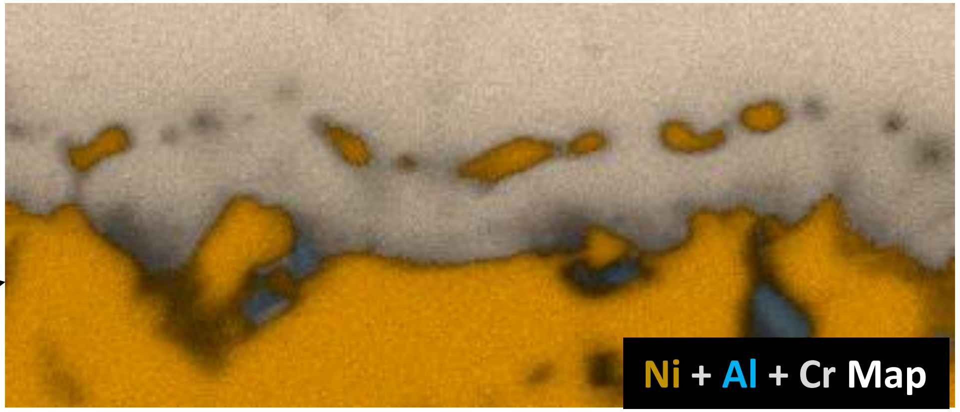
Microstructure: Typically 15-20 μm thick oxide scale is observed on the surface with additional oxygen intrusion of 1-1.5 grain diameter depth along the grain boundary.

Typical Example of high-resolution Imaging combined with EDS Spectroscopy in the SEM to characterize the extent of oxygen intrusion

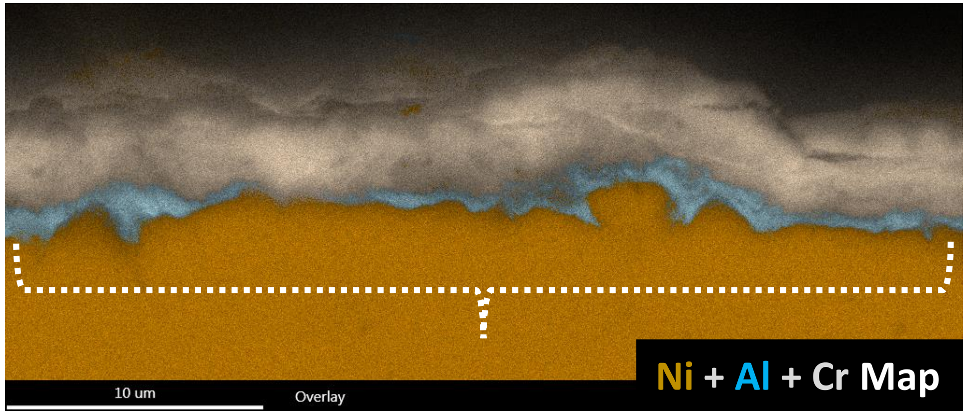
Alloy 282- Exposed at 925°C,1000 hrs
(without the protection from Al-rich oxide layer



Alloy 282- No Protection from Al-rich oxide layer



Alloy 224- Good Protection from Al-rich oxide layer



Aluminum rich oxide layer can be seen sandwiched between the bulk material.

Milestones

Date	Milestone	Status	Updated Target
2-1-2019	MS 1. ICME Integration Plan	Complete	
2-1-2019	MS 2. Sample Fabrication: High Temperature Oxidation Coupons	Complete	
9-1-2019	MS 3. Fabrication of microchannel-like prototype component	Delayed: Materials, COVID and Quintus partnership	11-30-2020
11-1-2019	MS 4. High temperature oxidation testing	Delayed	10-1-2020
6-1-2020	MS 5. High temperature creep testing of prototype component	Delayed	6-1-2021
9-30-2020	MS 6. Demonstration, verification and validation of model	Delayed	9-30-2021

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