Modeling Creep-Fatigue-Environment Interactions in Steam Turbine Rotor Materials for Advanced Ultrasupercritical Coal Power Plants

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imagination at work

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High temperature rotor application

HP/RHT Rotor

- High temperature steam
- High stress concentration at bucket connection

→ Creep-fatigue-environment interaction

- **DOE's goal: A-USC 1400˚F capability (5000 psi steam, 20+years)**
- **Candidate alloy: Alloy 282**

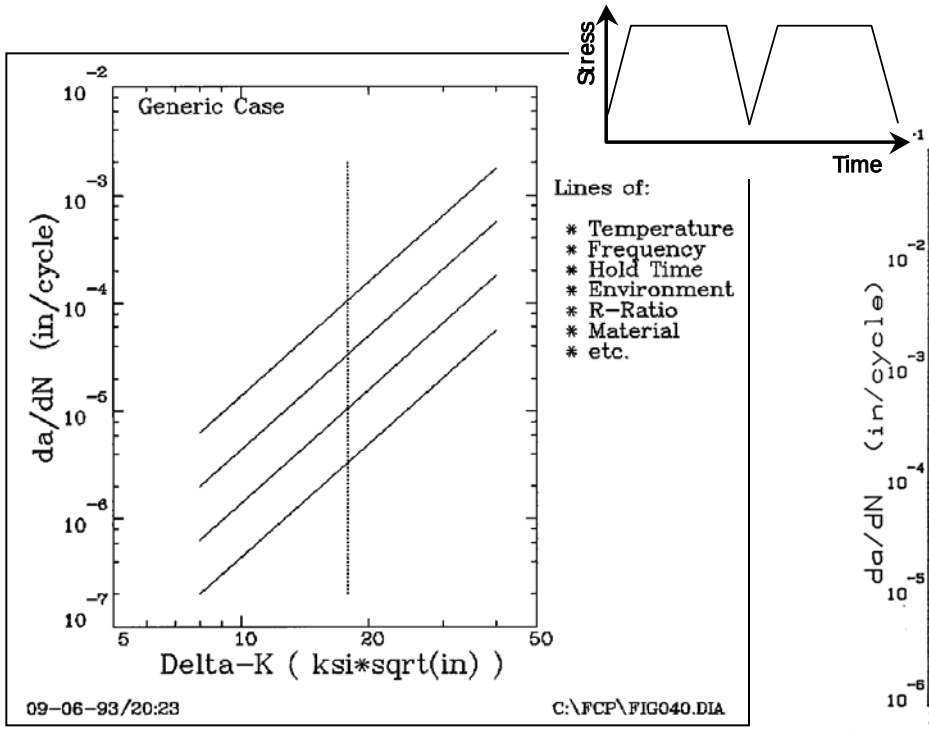
Overall goal and tasks of the program

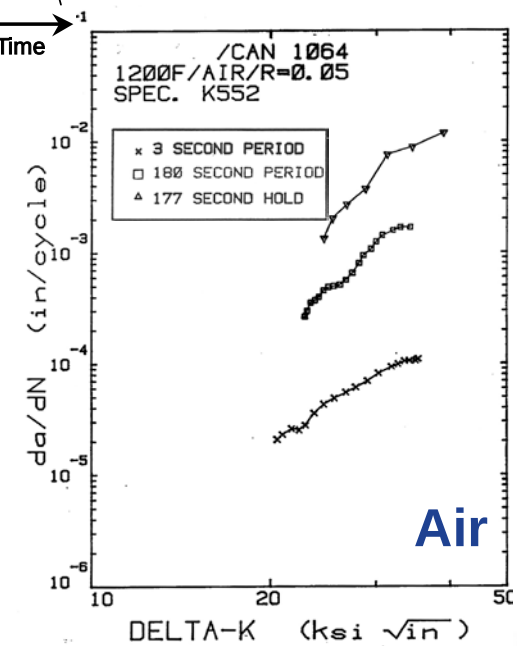
Creep-fatigue-environment interactions of Alloy 282

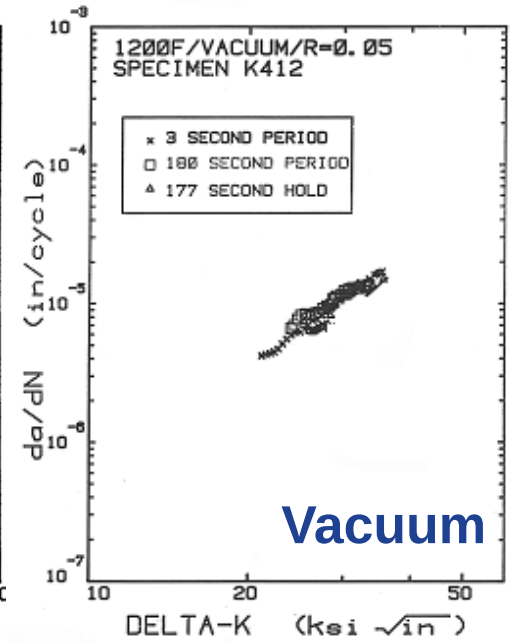
- Fatigue behaviors in steam and air environment
  - Hold-time fatigue experiment (Task 2)
  - Fundamental understanding at crack tip (Task 2,3)
  - Hold-time fatigue modeling (Task 6, 4)

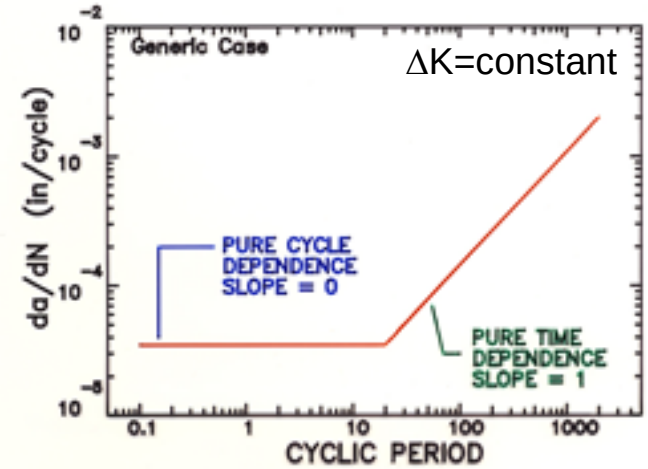
- Creep behaviors
  - Creep modeling & prediction (Task 5)
  - Long-term microstructure stability (Task 4)

Time dependent fatigue crack propagation





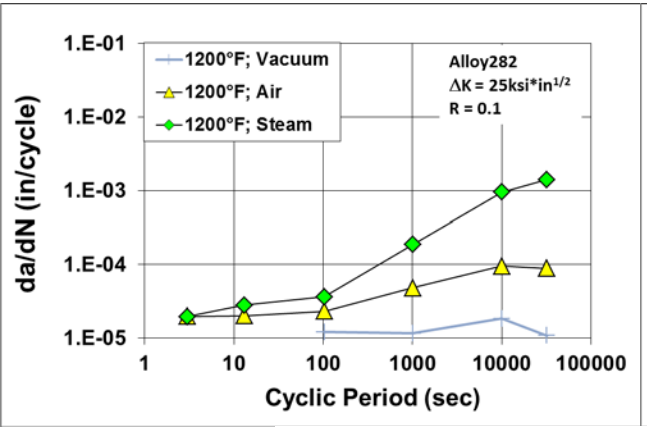




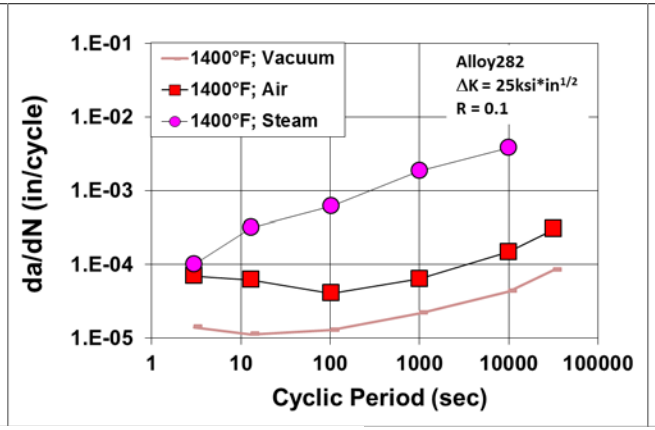
Environment-fatigue interaction dominates at *conventional* wheel stresses and temperatures

Alloy 282 hold time fatigue behavior

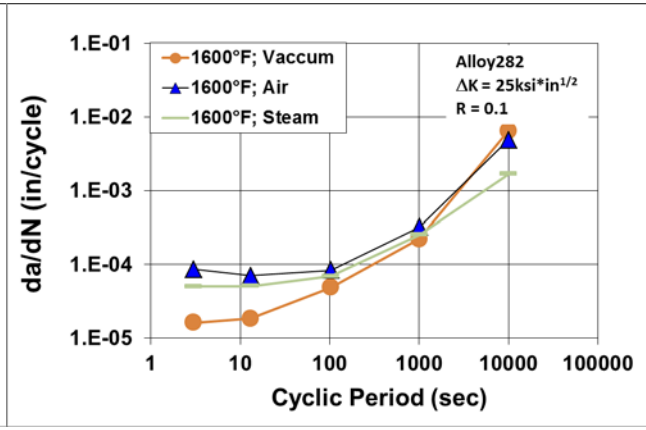
1200°F



1400°F



1600°F



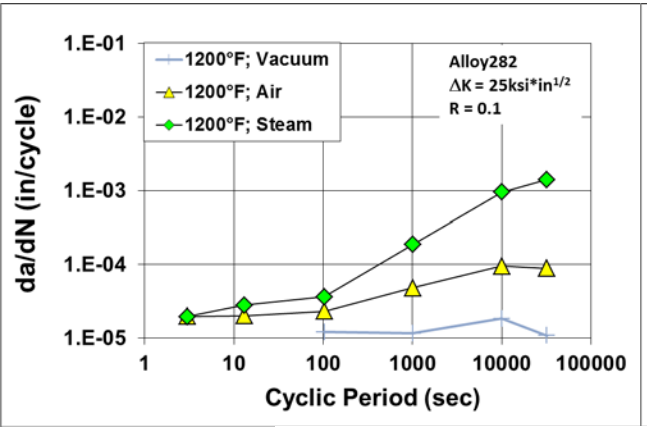
(—— Environment-Fatigue Interaction ——)

(– Environment-Creep-Fatigue –)

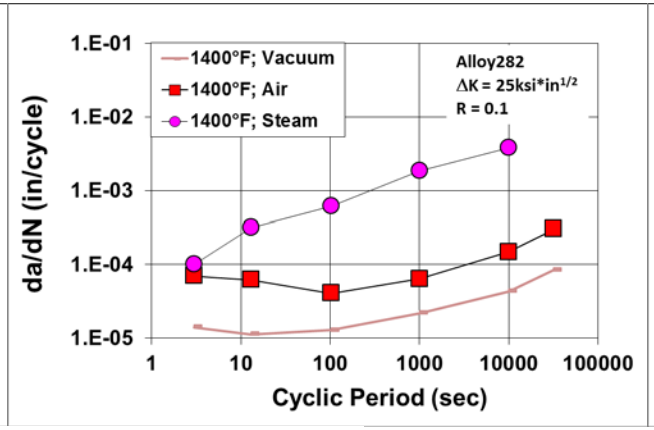
Convergence of air, steam, and vacuum data at 1600°F suggests pure creep-fatigue interaction. **<u>However</u>**, environment still plays a role

Alloy 282 hold time fatigue behavior

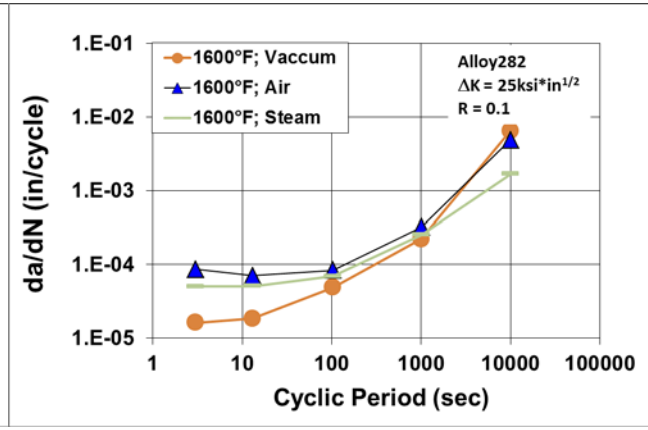
1200°F



1400°F

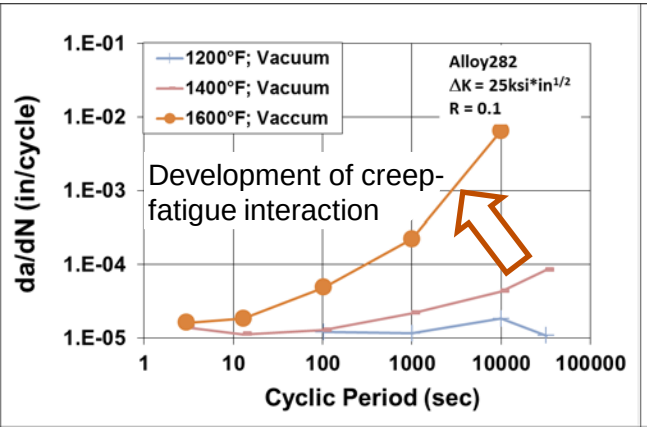


1600°F

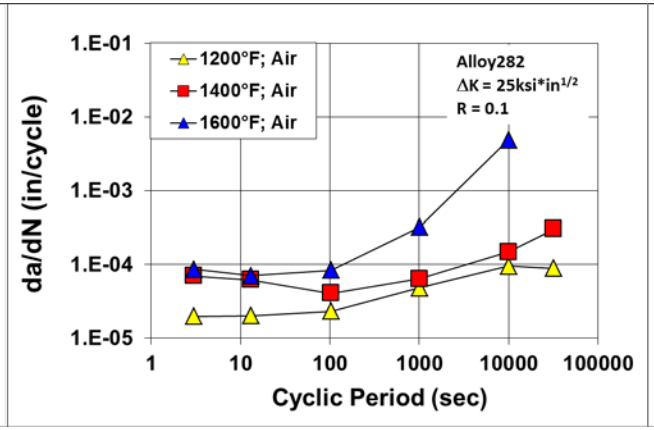


(— Environment-Fatigue Interaction —) (— Environment-Creep-Fatigue —)

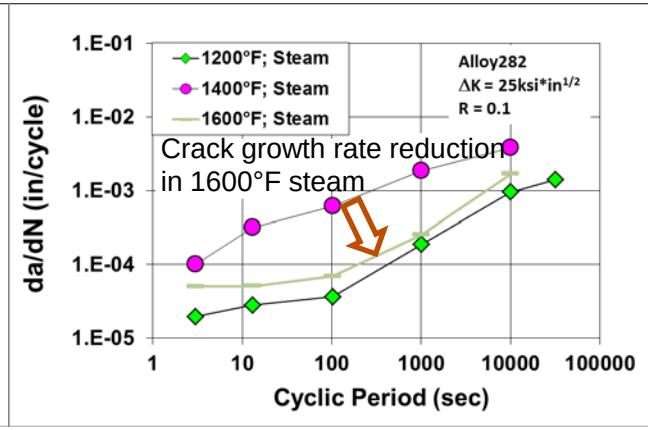
Vacuum



Air

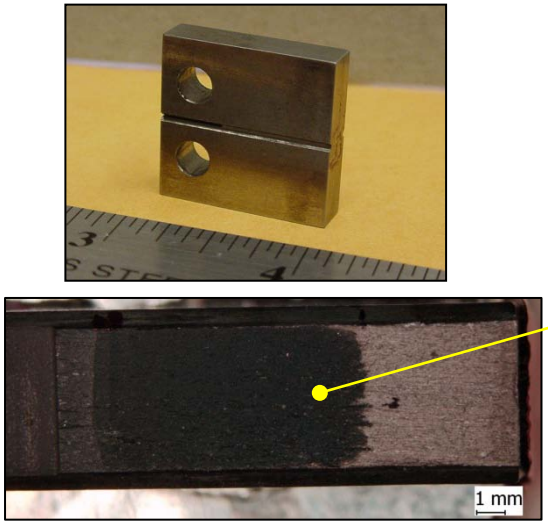


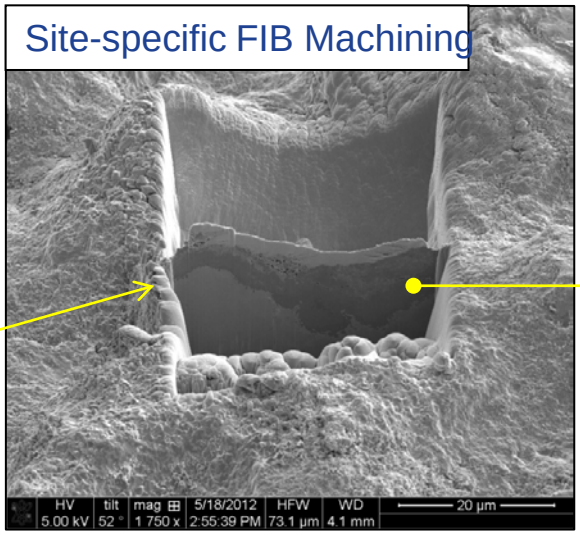
Steam

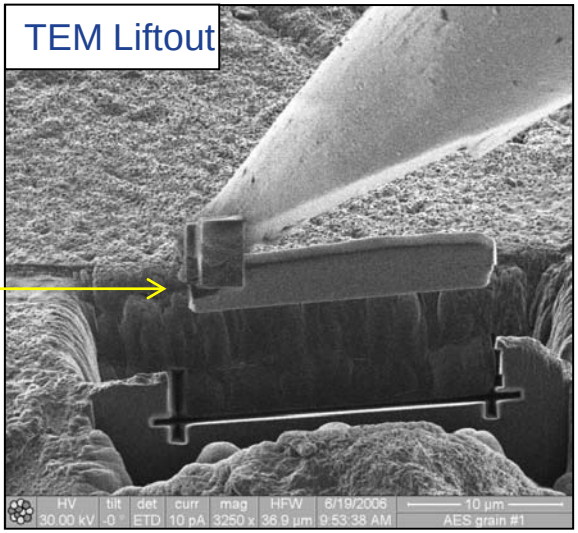


(— Combination of environmental- and creep-fatigue interactions —)

Alloy 282 fracture surface oxide characterization







"Transient" oxidation

Rapid formation

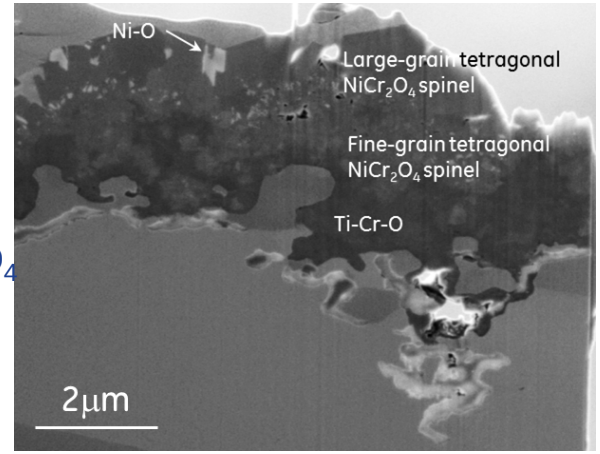
↓

$NiO+Cr_2O_3 = NiCr_2O_4$

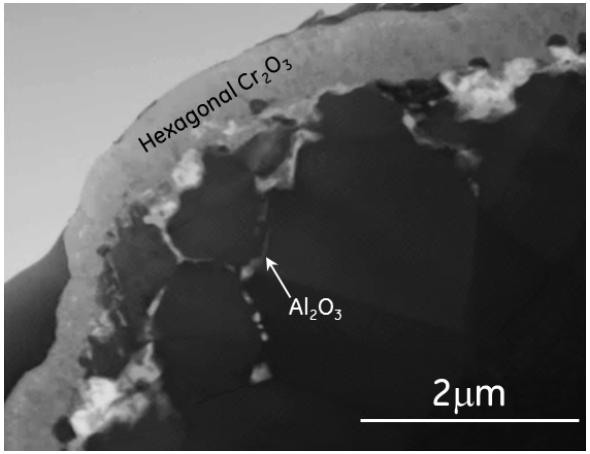
↑

Slow forming

1400°F Air



1400°F Steam



Selective oxidation (Cr_2O_3 formation) is promoted by reduced oxygen partial pressure

Fracture surface oxidation characteristics differ in air and steam

Crack tip oxide evaluation: 1400˚F Air

X-ray maps: O-Ti-Al-Ni

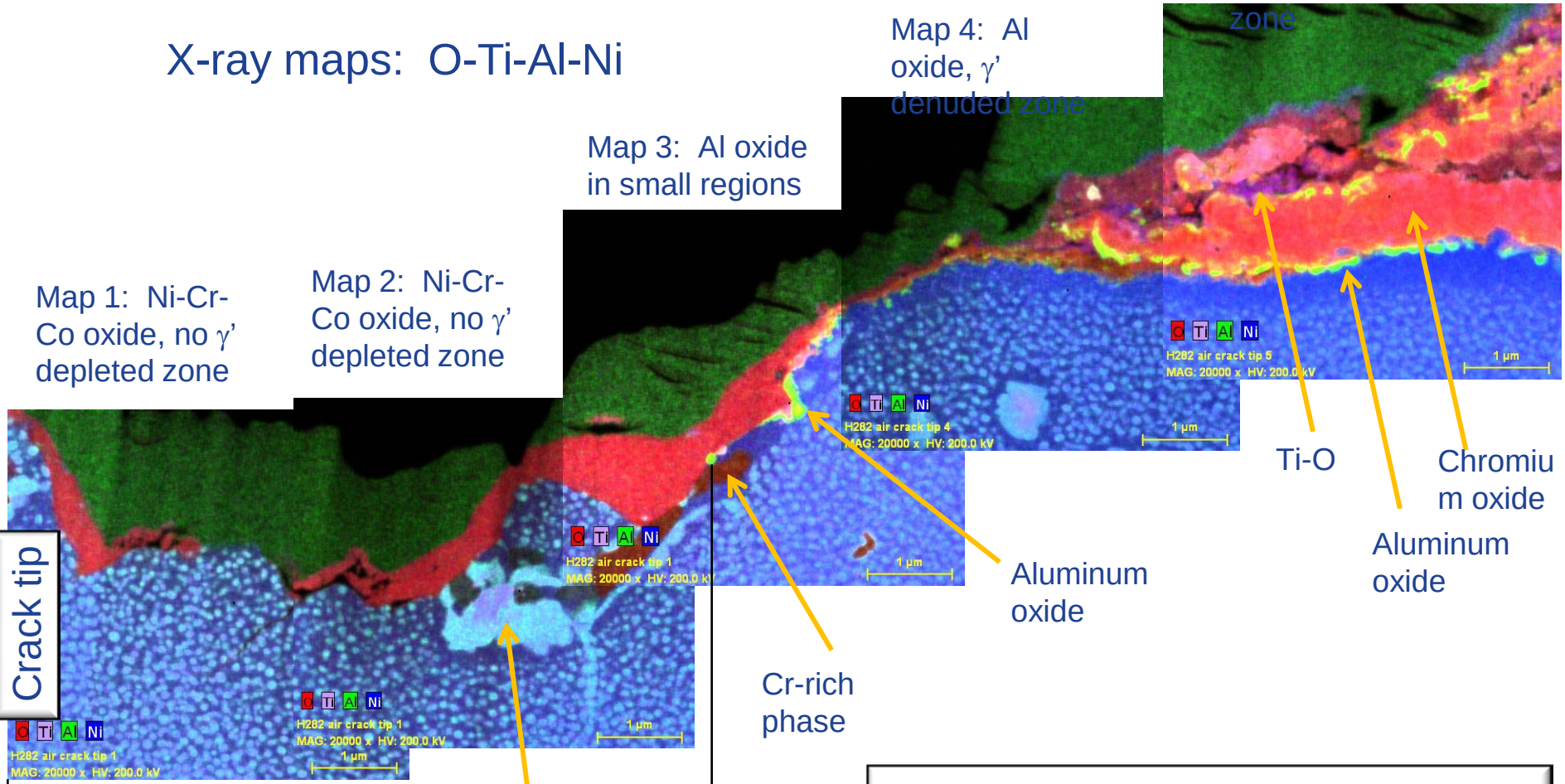
Map 1: Ni-Cr-Co oxide, no γ' depleted zone

Map 2: Ni-Cr-Co oxide, no γ' depleted zone

Map 3: Al oxide in small regions

Map 4: Al oxide, γ' denuded zone

Map 5: Al oxide, Ti oxide, Cr oxide regions, γ' denuded zone



9µm (~10 hours of growth) to first Al_2O_3

Al_2O_3 and Cr_2O_3 formation is delayed at the crack tip under 1400°F air conditions

imagination at work

Crack tip oxide evaluation: 1400˚F Air

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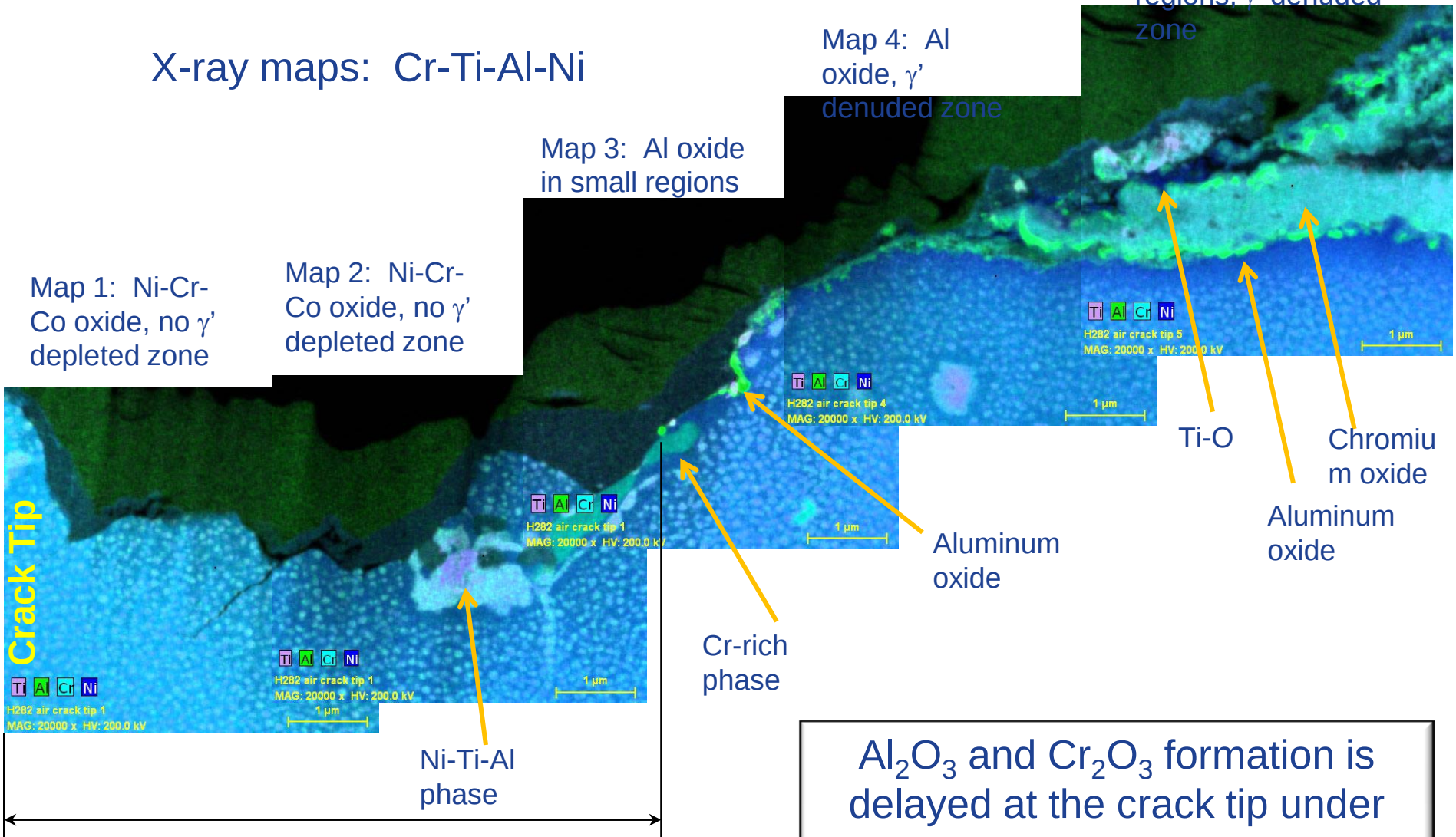

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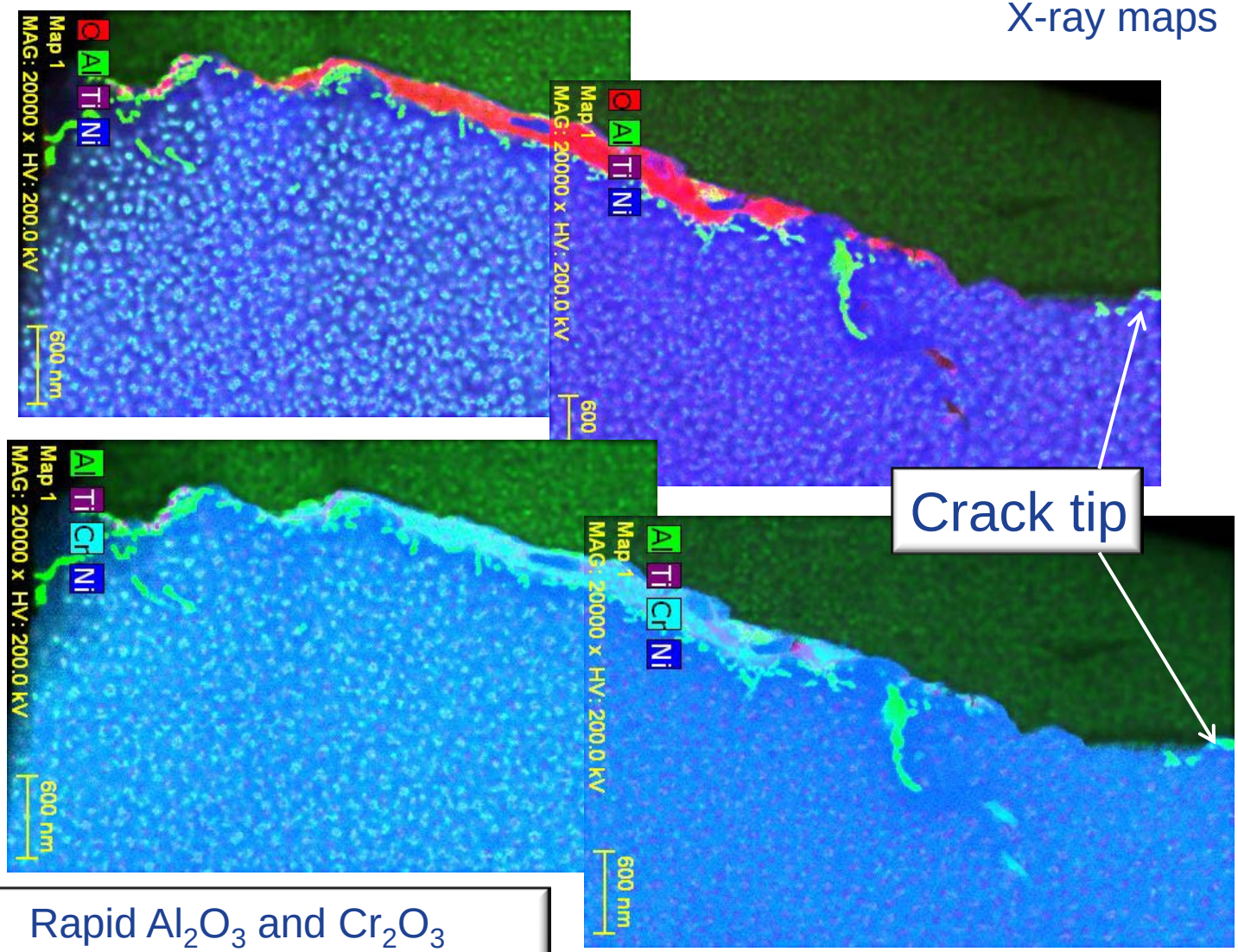
imagination at work

Crack tip oxide evaluation: 1400˚F Steam

X-ray maps

O-Ti-Al-Ni

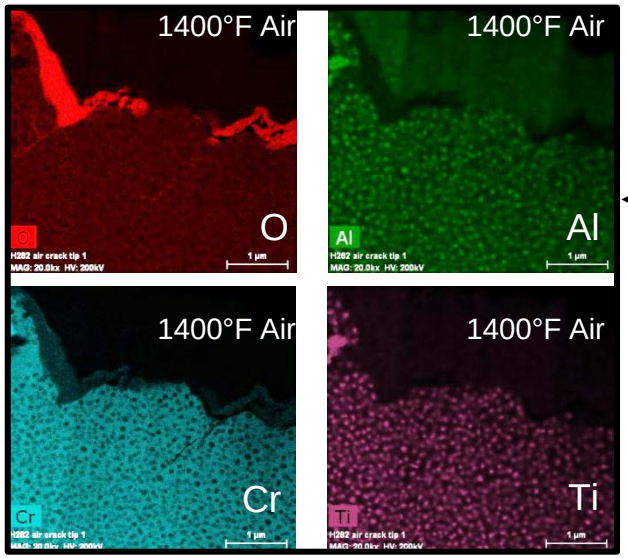
Cr-Ti-Al-Ni



Rapid Al_2O_3 and Cr_2O_3 formation kinetics in 1400°F steam

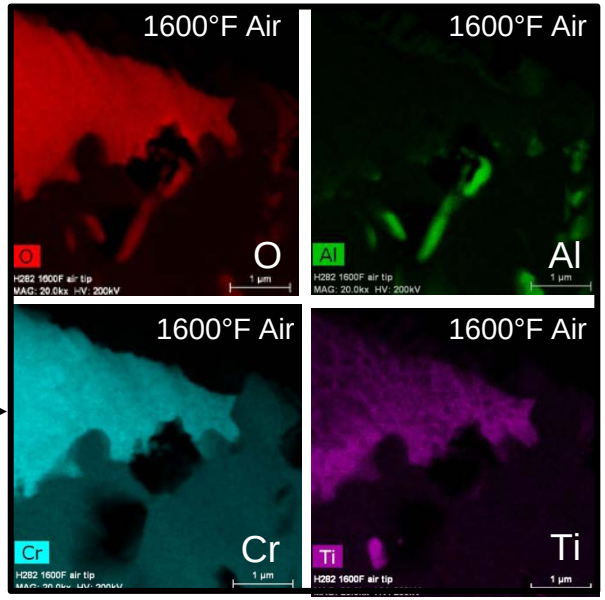
**Crack tip gamma prime depletion

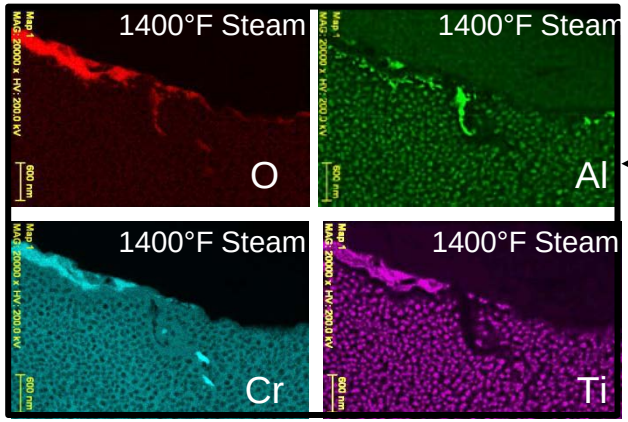
Crack tip oxide characteristics



No crack tip Al_2O_3 or Cr_2O_3

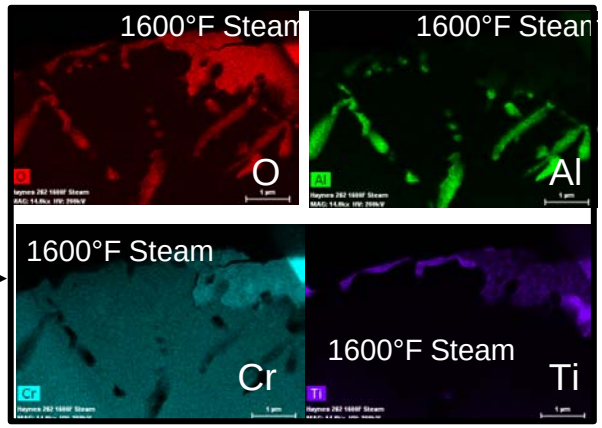
Crack tip Al_2O_3 or Cr_2O_3





Crack tip Al_2O_3 or Cr_2O_3

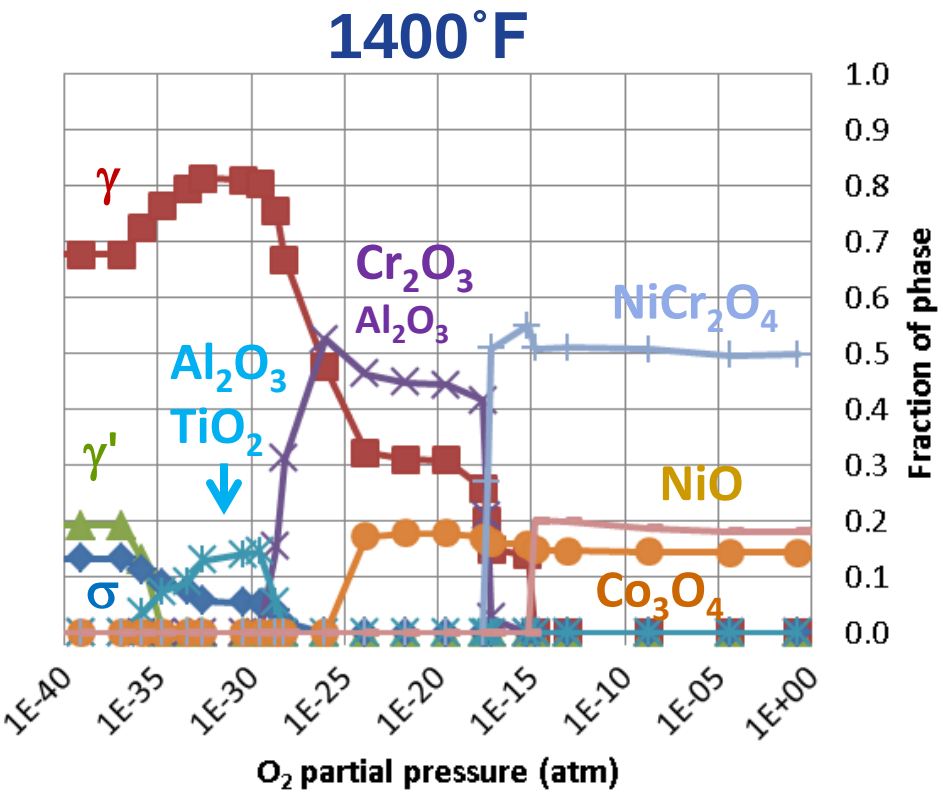
Crack tip Al_2O_3 or Cr_2O_3

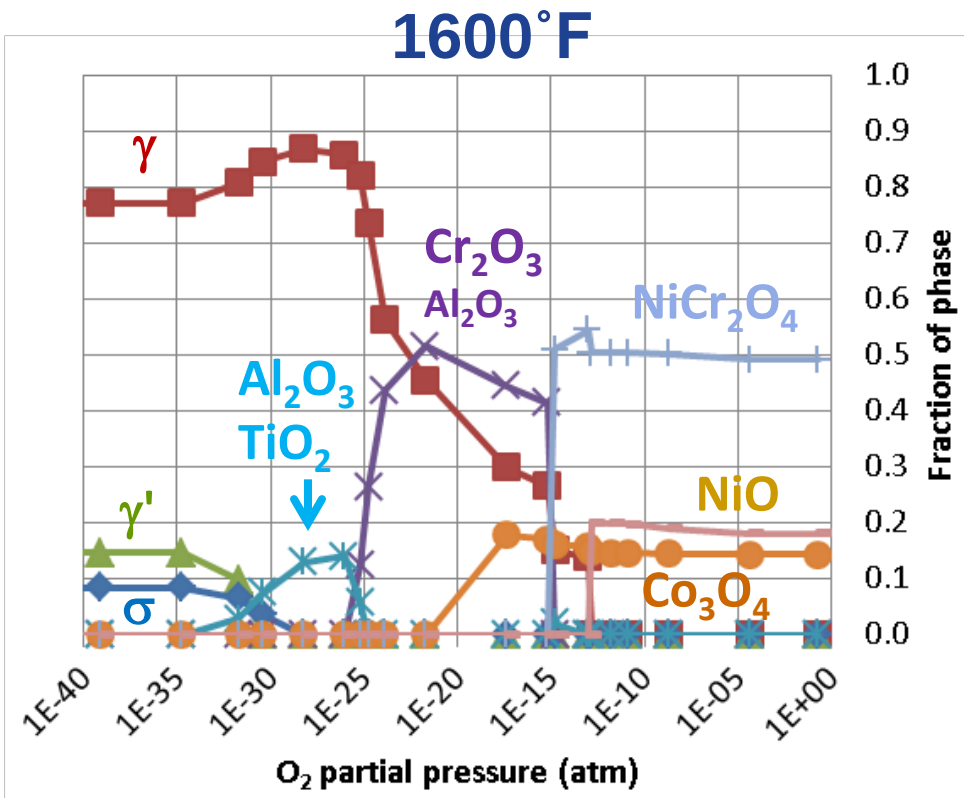


Depth of gamma prime depletion larger at 1600°F

Local crack tip oxidation resistance **may** correlate crack growth resistance

Thermodynamic understanding of oxides in Alloy 282



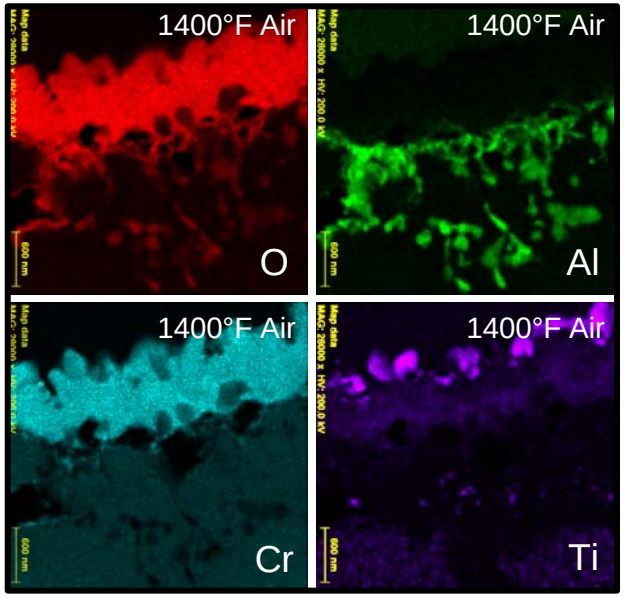


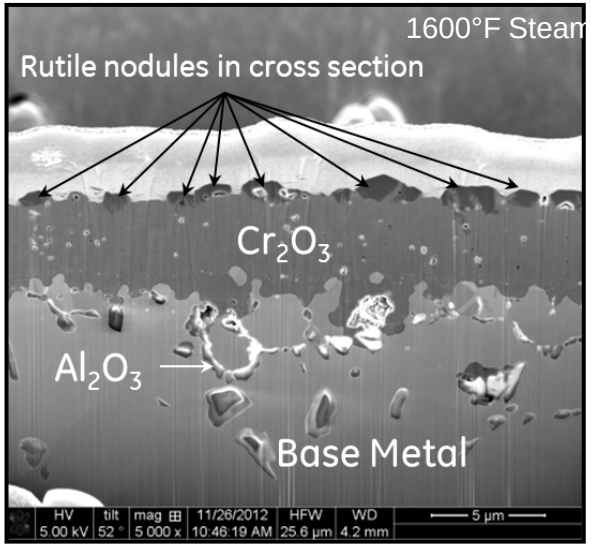
pO2 ➔
- Environment
- Depth from surface

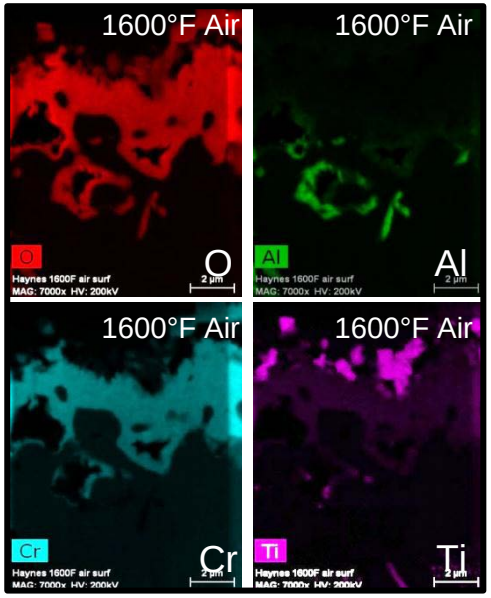
↓ pO_2 : NiO, $NiCr_2O_4$ & Co_3O_4 spinel ➔ Cr_2O_3 ➔ Al, Ti oxides (γ' dissolution)

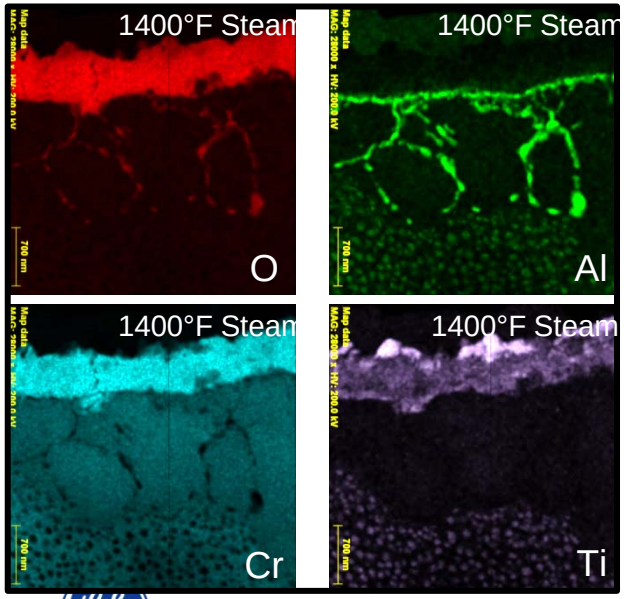
↑ T : as if environment pO_2 is lowered

Free surface oxide characteristics





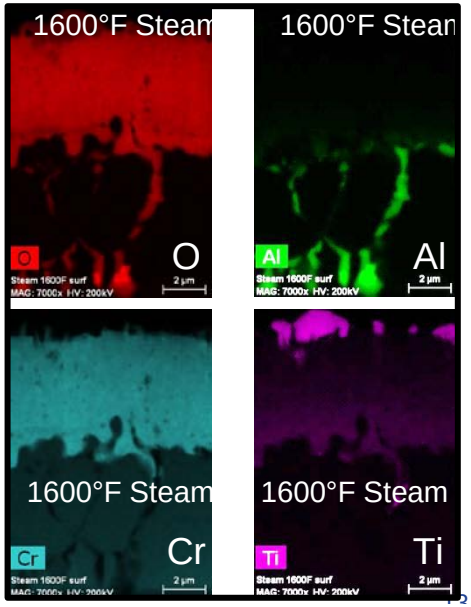




Free surface oxide characteristics similar in air and steam at 1400°F and 1600°F

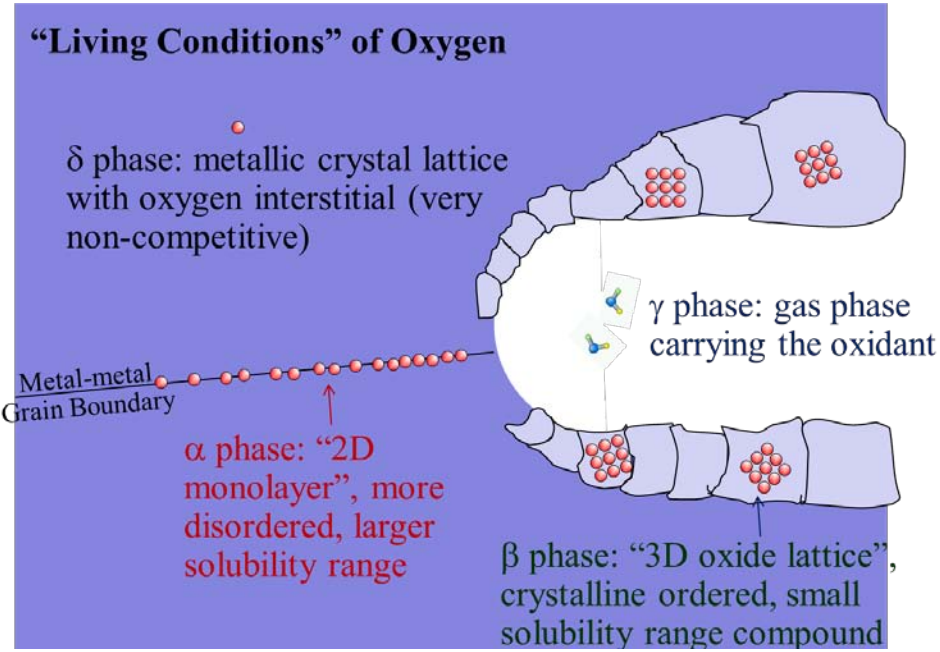
- Al_2O_3 internal oxidation
- Sub-surface gamma prime depletion
- Hexagonal Cr_2O_3
- Free-surface Ti-rich oxide

Bulk oxidation resistance **does not** correlate crack growth resistance



Depth of gamma prime depletion larger at 1600°F

Grain boundary – oxygen interaction micro-mechanisms



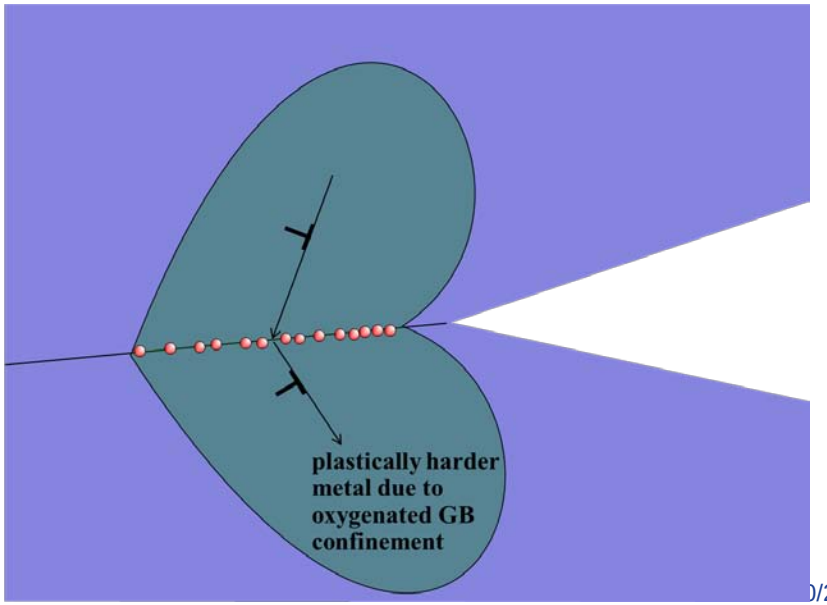
Our DFT calculations so far have not shown favorable thermodynamics for "α phase" formation in Ni GBs…

But, if it does exist, there will be two mechanical effects on GB:

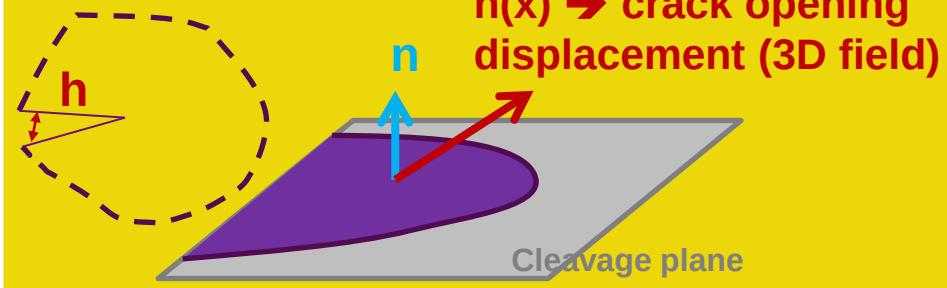
(a) Lower the cohesion of metal-metal GBs (by up to ~50%)

(b) Make GBs more difficult to transmit dislocations, which plastically hardens the surrounding metal

This nonlocal or confinement effect on metal plasticity is more difficult to model (Uchic, Dimiduk, Florando, Nix, Science 305 (2004) 986) than effect on local GB decohesion



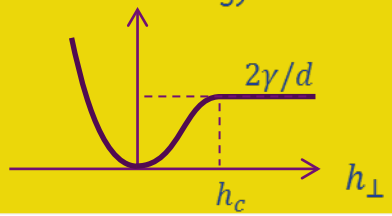
Modeling crack propagation with phase field method



Total energy driven:

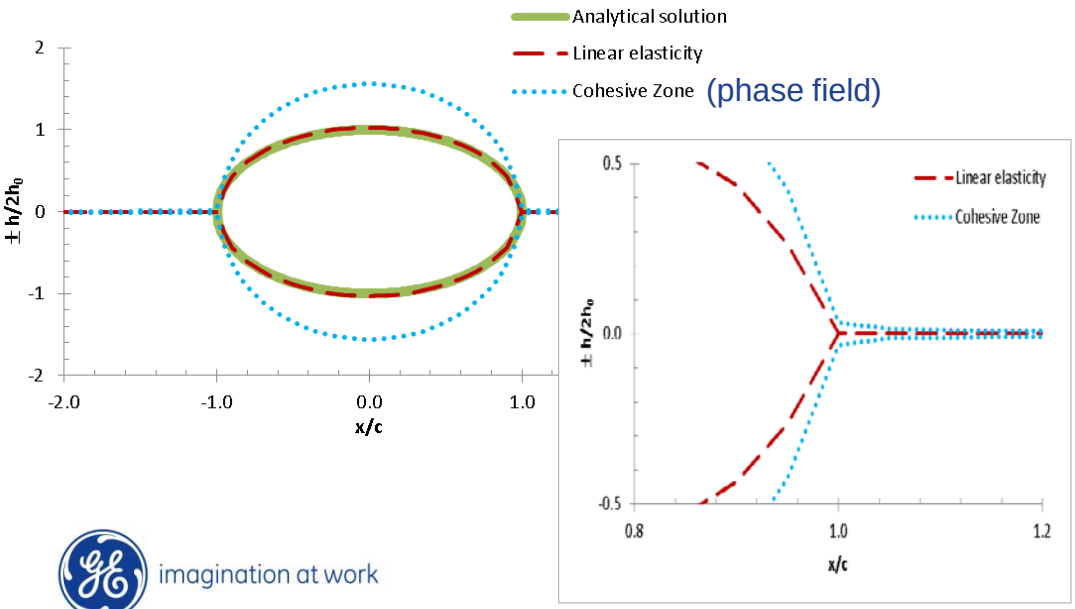
$$\text{"rate"} \propto -\frac{\delta\left[E^{coh}+E^{el}+E^{gr}+W^{appl}\right]}{\delta \mathbf{h}(\mathbf{x})}$$

Cohesion energy: E^{coh}

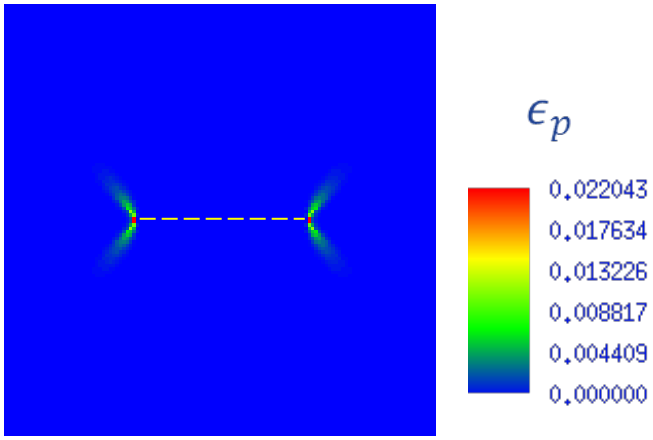


(Yu Wang et al, 2002)

Compare crack profiles



Incorporate von Mises yield based plasticity



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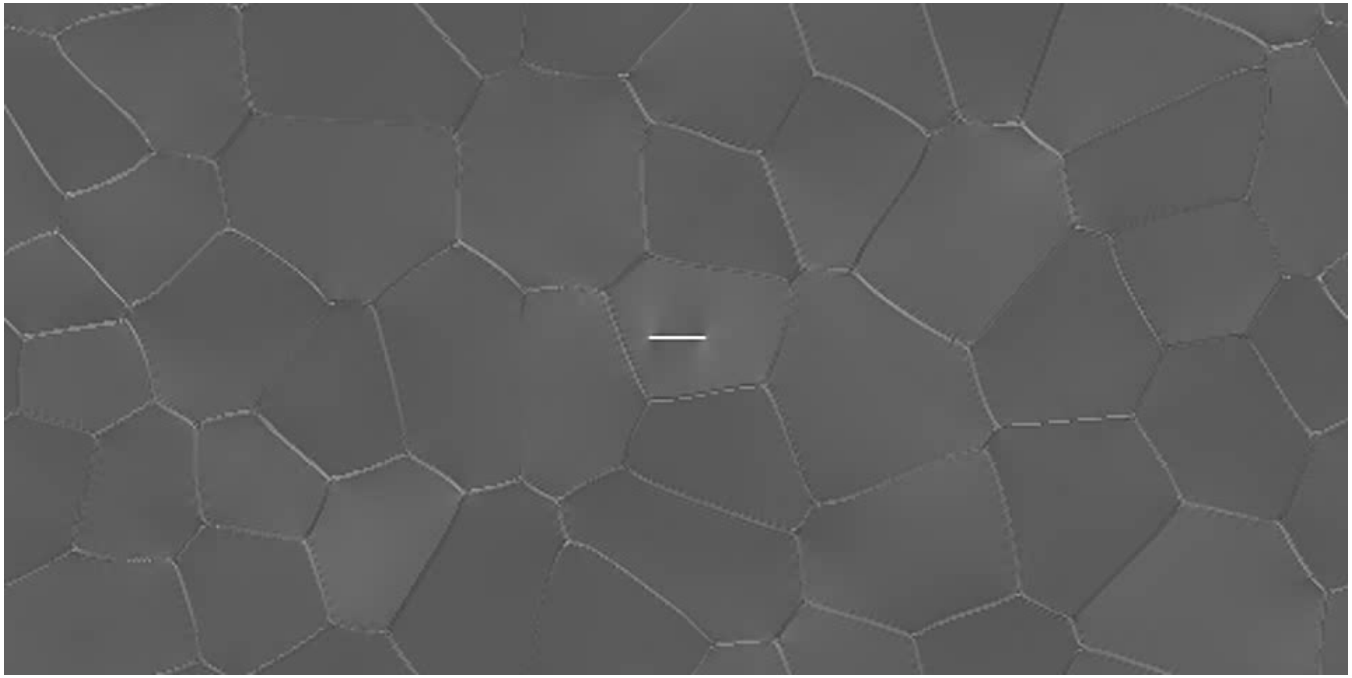
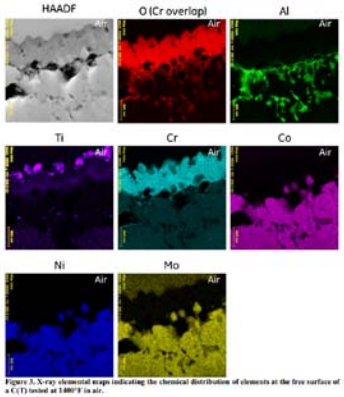
Modeling crack propagation in polycrystal (preliminary)

- **Aim to incorporate GB-O interactions**
- **Grain boundaries treated with lower cohesive energy**
- **Brittle cracking (no plastic yielding yet)**
- **Static constant tensile load, near half ideal cohesive strength**



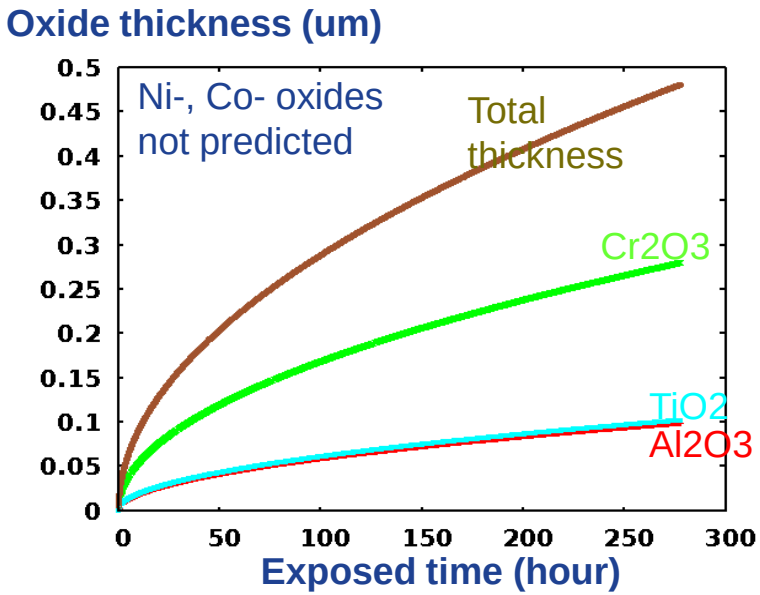
Diffusion-oxidation kinetics modeling

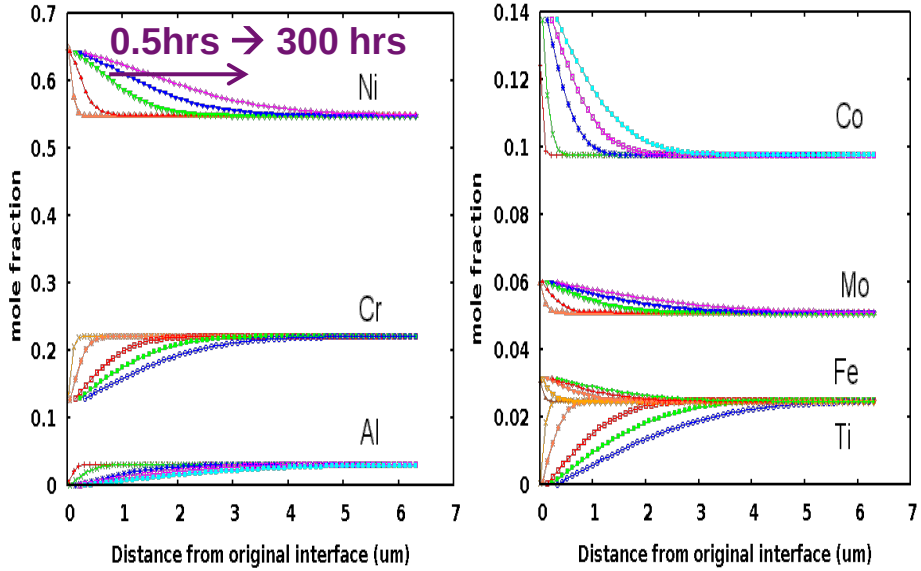
- **Selection of oxide phase by current equilibrium pO_2 at oxide-metal interface**
- **Elements' diffusivity and activity in metal from CALPHAD database; lack the data in oxides**
- **Simplified oxide growth (parabolic) law**
- **Multi-element diffusion in metal substrate**



Overall oxidation rate $k = 2.3 \times 10^{-7} \mu m^2/s$ estimated from 1400°F air exposed specimen

To be incorporated to phase field crack modeling





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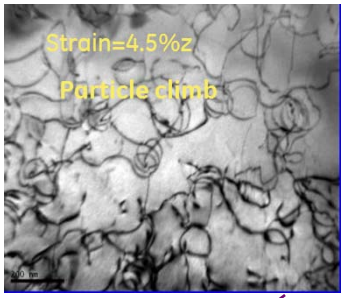
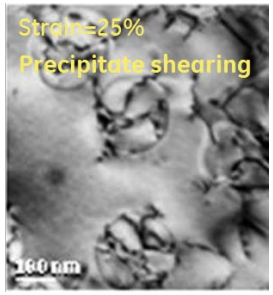
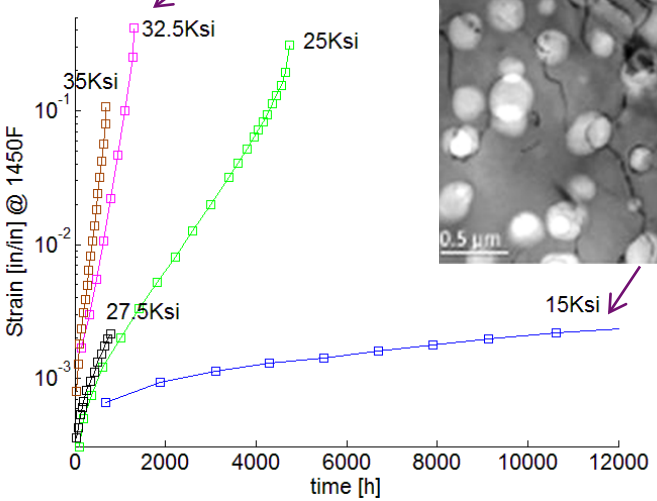
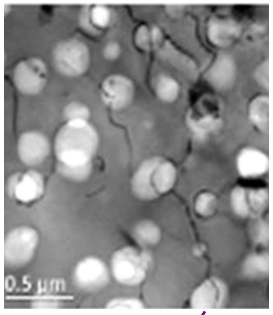
Creep modeling for Alloy 282

- **To develop a mechanism-based creep model for Alloy 282 under A-USC conditions**









Dislocation climb-bypass γ' observed as a main deformation mode in 282

Total creep ← effect of dislocation and diffusion creep

$$\varepsilon^{creep} = \varepsilon^{disloc} + \varepsilon^{diffusion}$$

Dislocation climb-bypass (Dyson, 2009)

$$\dot{\varepsilon}^{disloc} = A\rho f(1-f)\left(\sqrt{\frac{\pi}{4f}} - 1\right)\sinh\left(C\frac{\sigma_{eff} - \sigma_B - \sigma_0}{MkT}\lambda b^2\right)$$

$$\sigma_{eff} = \frac{\sigma_{applied}(1+\varepsilon)}{1 - D_s}$$

$$\dot{\sigma_B} = E\frac{f}{1-f}\dot{\varepsilon}^{disloc}\left(1 - \frac{\sigma_B}{2f/(1+2f)\sigma_{eff}}\right)$$ primary creep

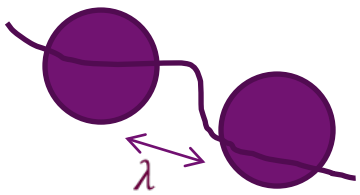
$$\dot{\rho} = F(\rho_f - \rho)\dot{\varepsilon}^{disloc}$$ primary/secondary creep

$$\dot{D_S} = B\dot{\varepsilon}^{disloc}$$ tertiary creep and creep damage

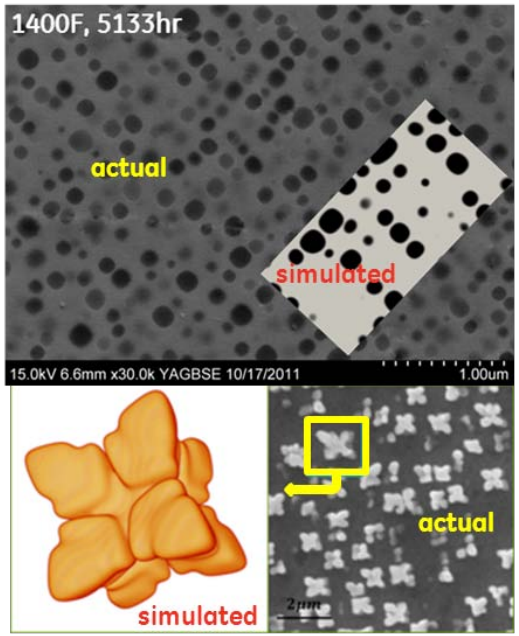
$$\dot{\varepsilon}^{diffusion} = D\frac{\sigma\Omega}{d^2 k_B T}$$ **Diffusion creep**

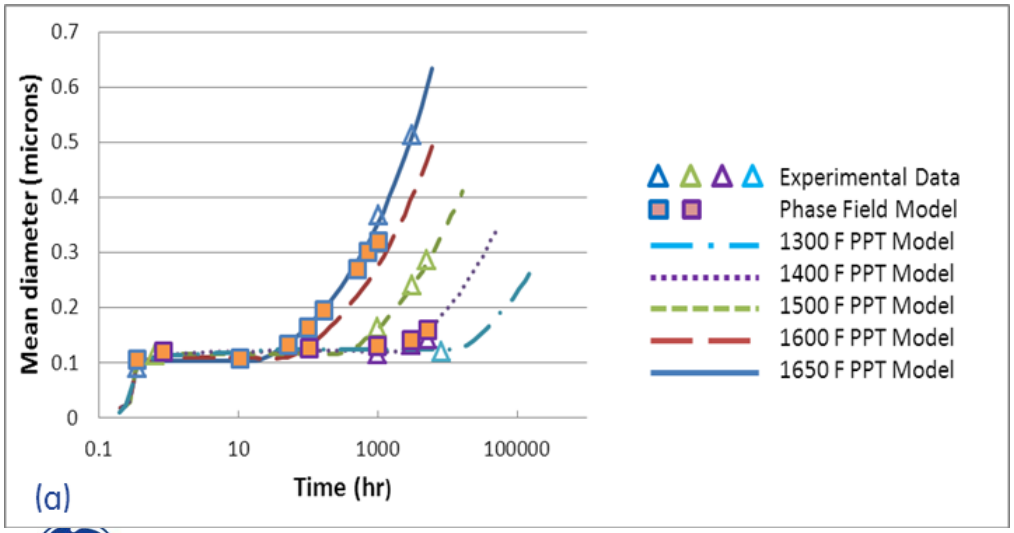
f, λ : vol. fraction and spacing of γ' precipitates

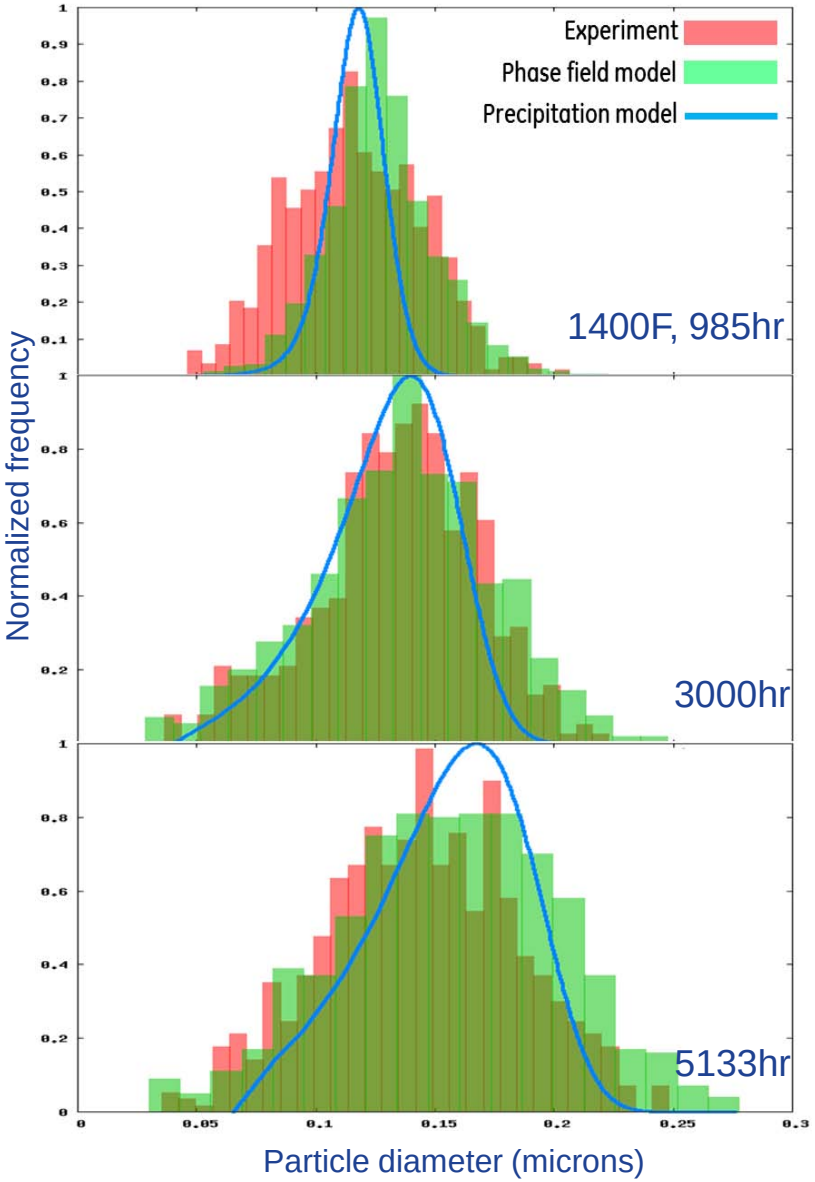
Incorporate γ' microstructure change



$\sigma \sim 1/\lambda$



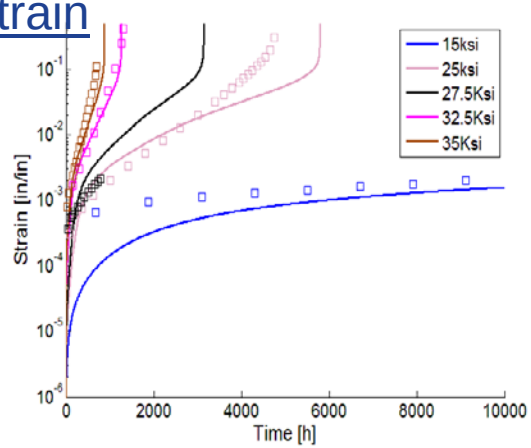


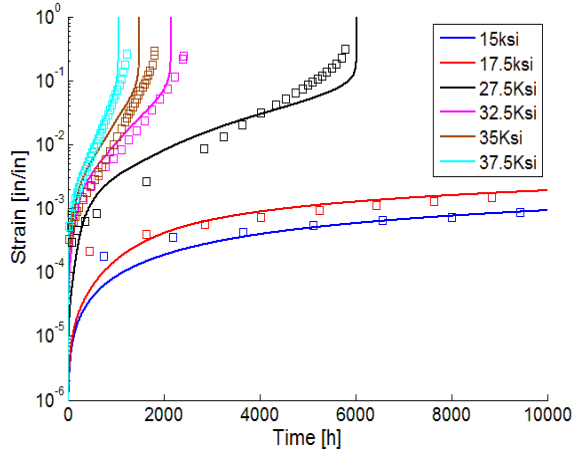


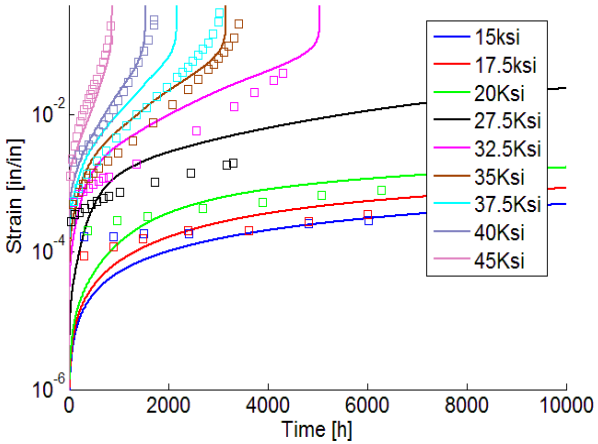
Prediction of creep strain and strain rate of Alloy 282

(Boxes are experimental data)

Strain





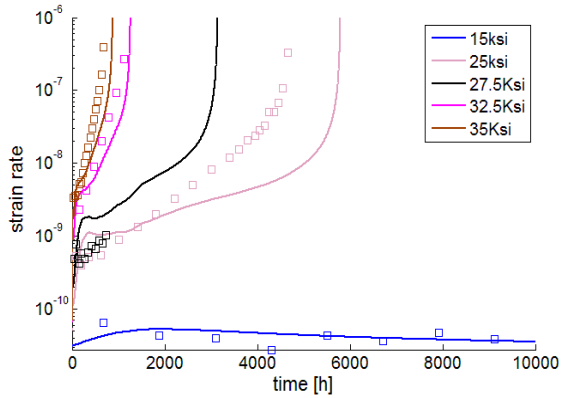


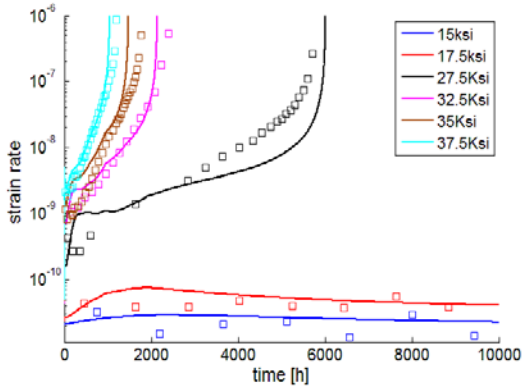
1450F

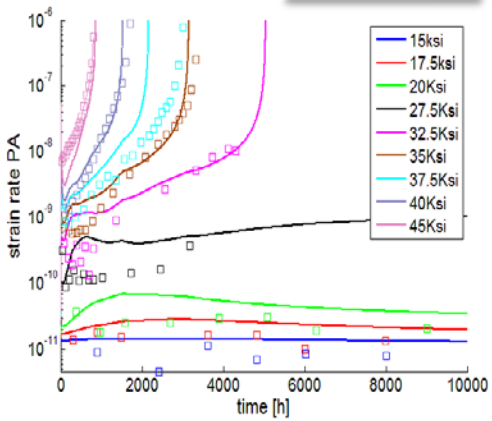
1425F

1400F

Strain rate



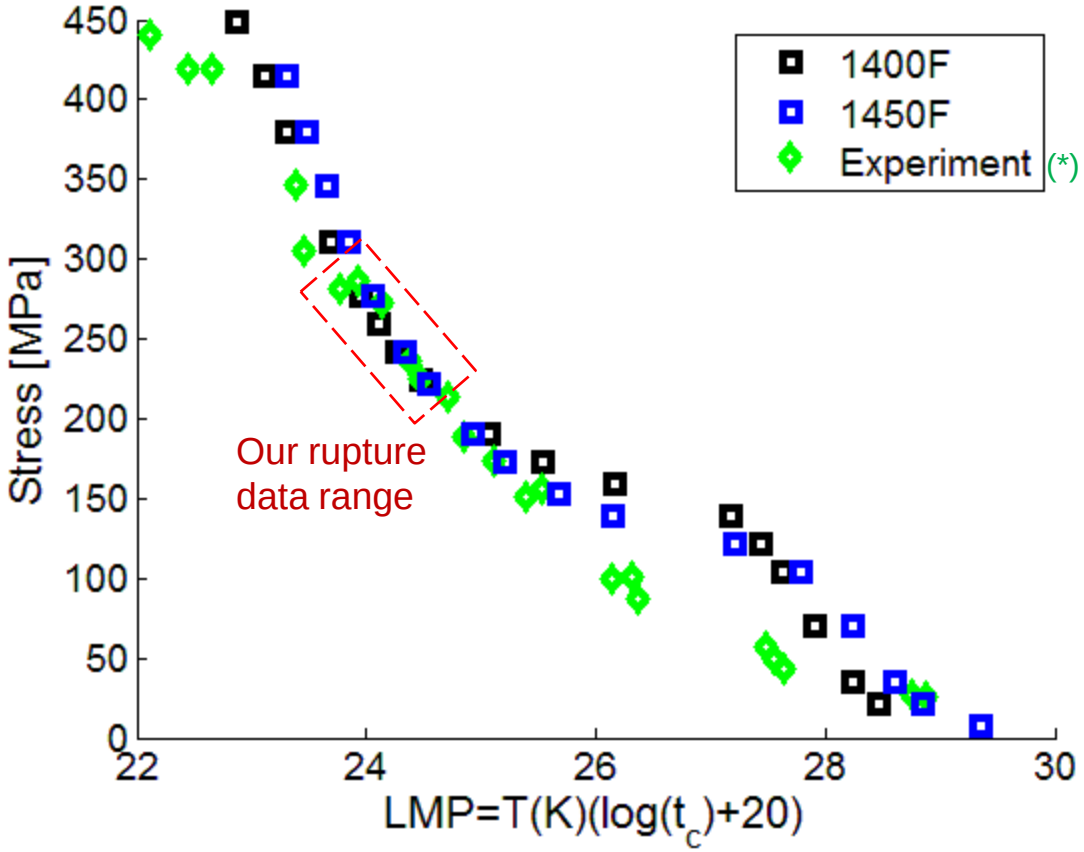




Good agreement with creep data for a broad range of stress and temperature

imagination at work

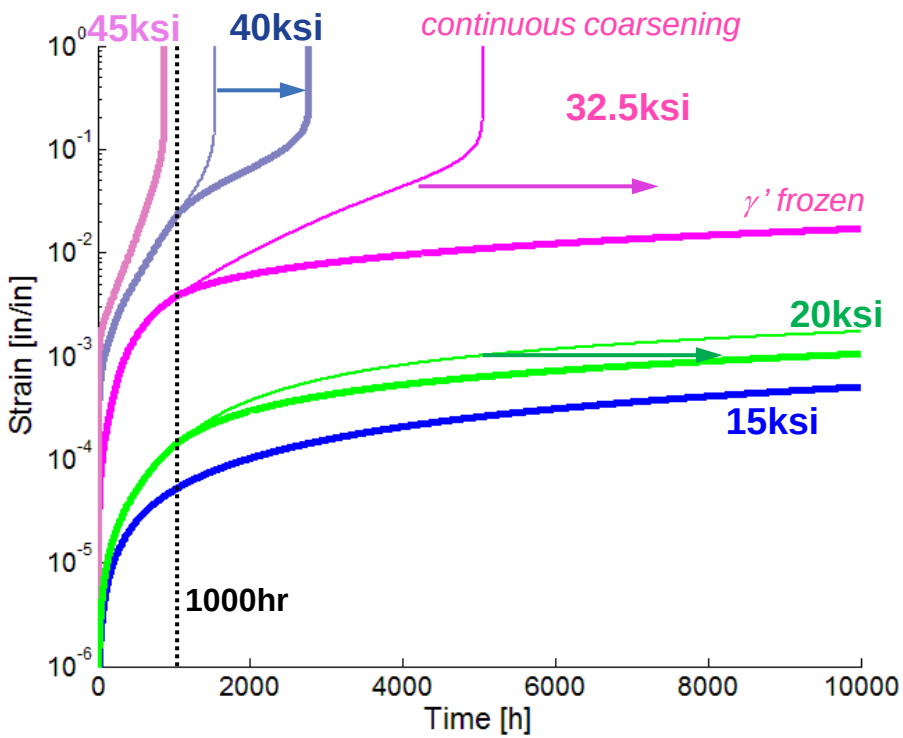
Prediction of creep rupture

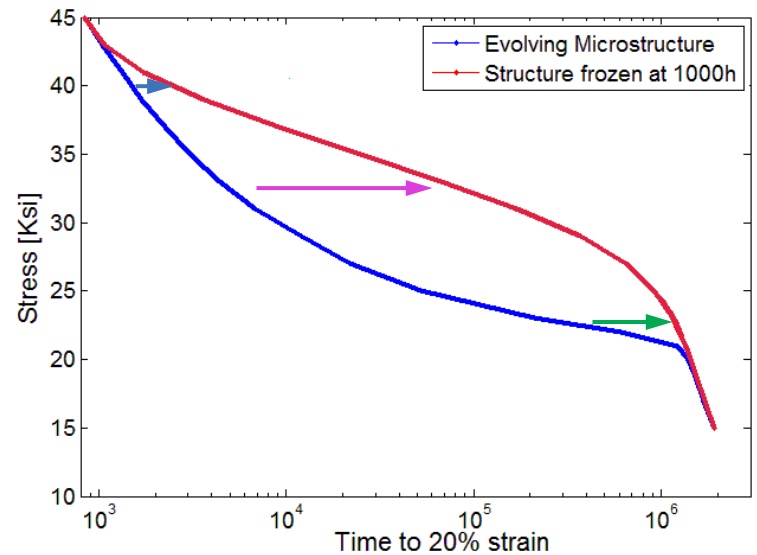


* Long-term creep test: Mike Santella, ORNL, 24th Annual Conf. Fossil Energy Matl. Pittsburgh, PA, 2010

Sensitivity to γ' microstructure evolution in Alloy 282

- **Continuous coarsening vs. γ' frozen at 1000hr**

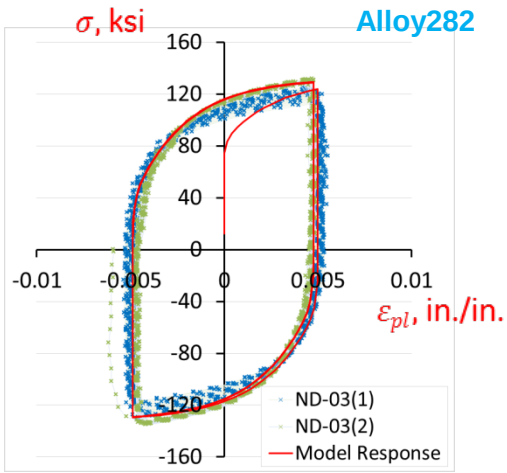




Sensitivity to γ' size greatest at intermediate stresses, and negligible below 15ksi (~100MPa)

Multiscale modeling for Alloy 282 - Fatigue and confined crack tip plasticity (CCTP)

2 Chaboche material model calibration



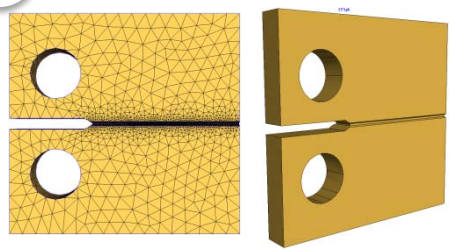
$$\frac{d\underline{\underline{\varepsilon}}}{dt} = f(\underline{\underline{\sigma}},\ldots)$$

1 Test 1: Round-bar LCF testing

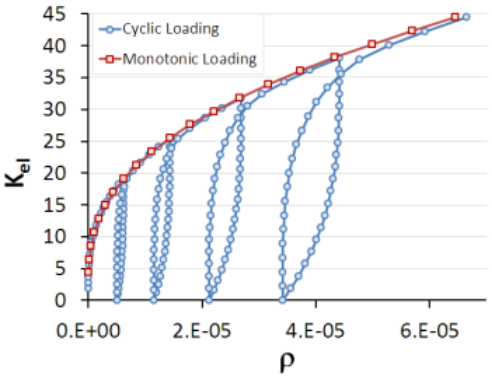
Identify material's cyclic, elastic-plastic response

imagination at work

3 FE simulations on CT model



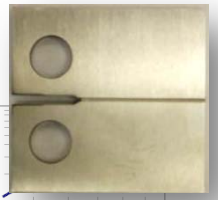
4 Crack tip plasticity evolutions to calibrate the



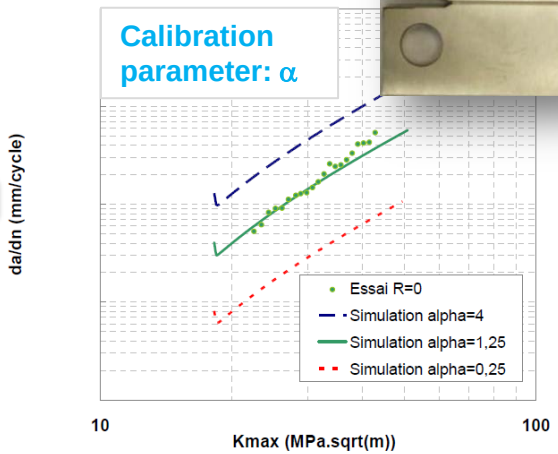
$$\frac{d\rho}{dt} = g(K_I,\ldots)$$

Goal: Fatigue crack modeling that incorporates the effect of load history, environment, and creep

5 Test 2: FCG test to calibrate da/dN curves[1]



Calibration parameter: α



6 Crack propagation simulation[1]

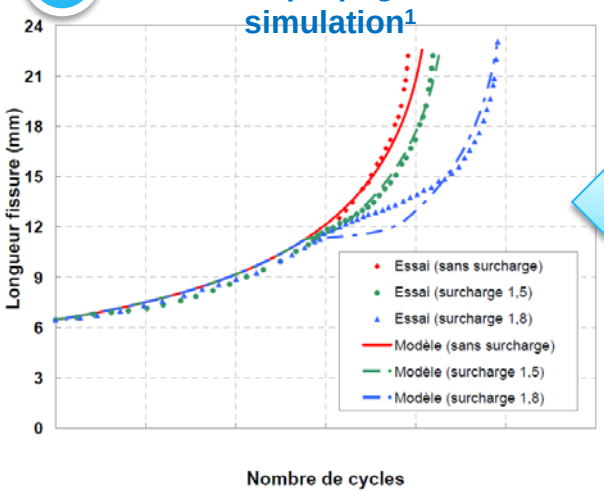
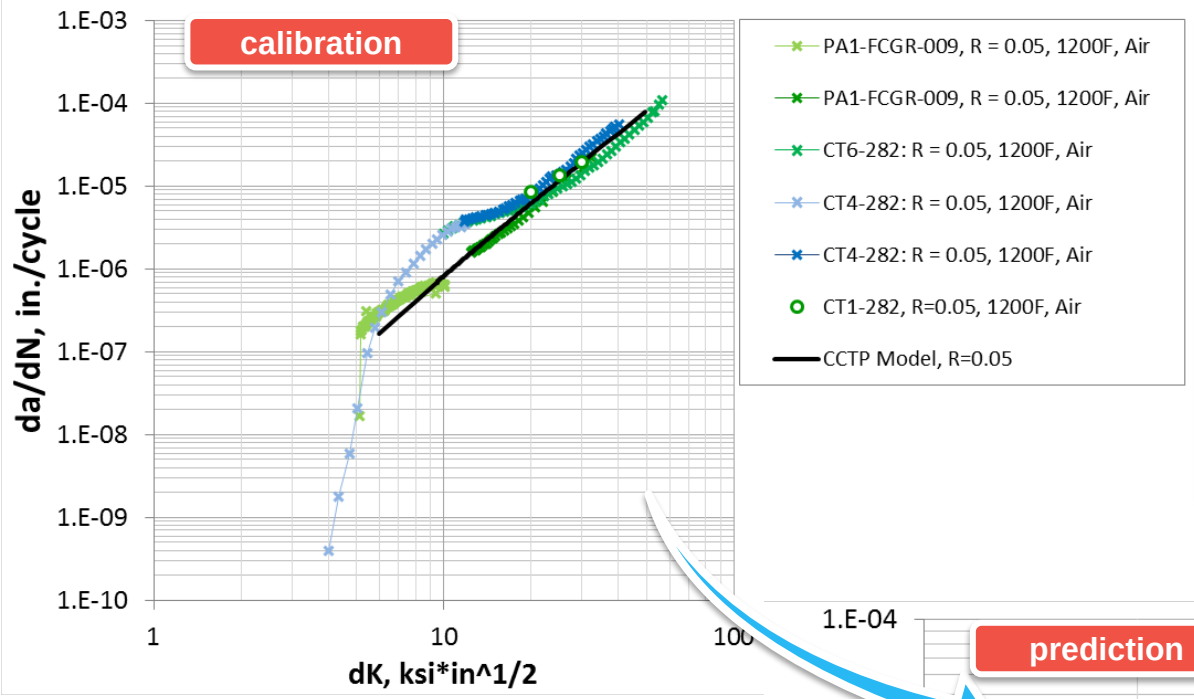


Figure 2-60. Comparaison essai-calcul pour des surcharges simples

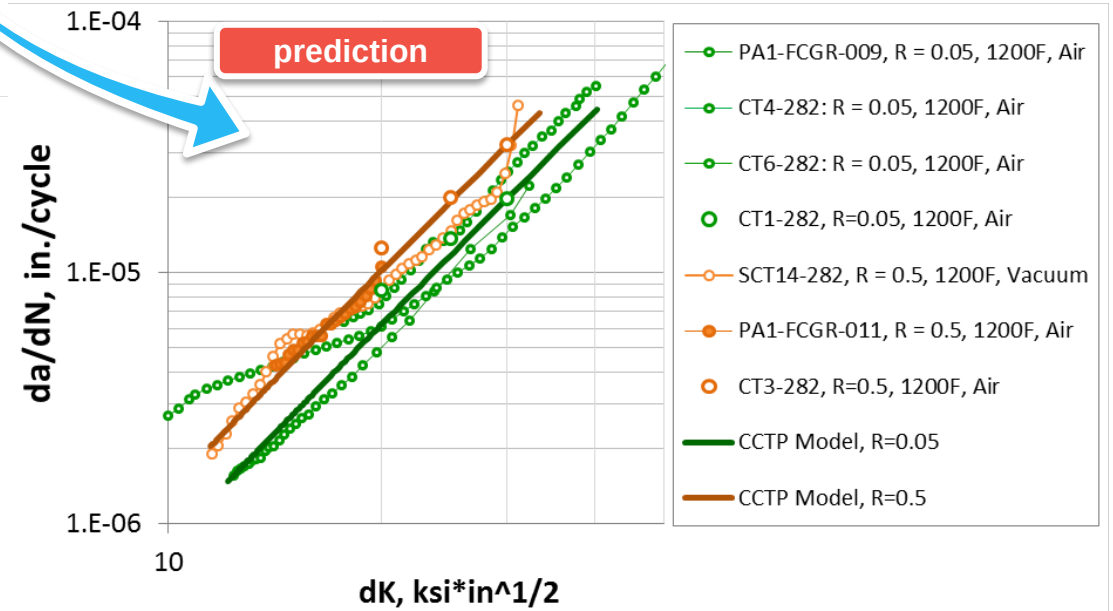
1. R. Hamam, S. Pommier F. et.al IJF 2007, 29: 1634-1646

Model calibration/prediction at 1200˚F for Alloy 282



- Calibration to load ratio R=0.05
- The slope predicted correctly

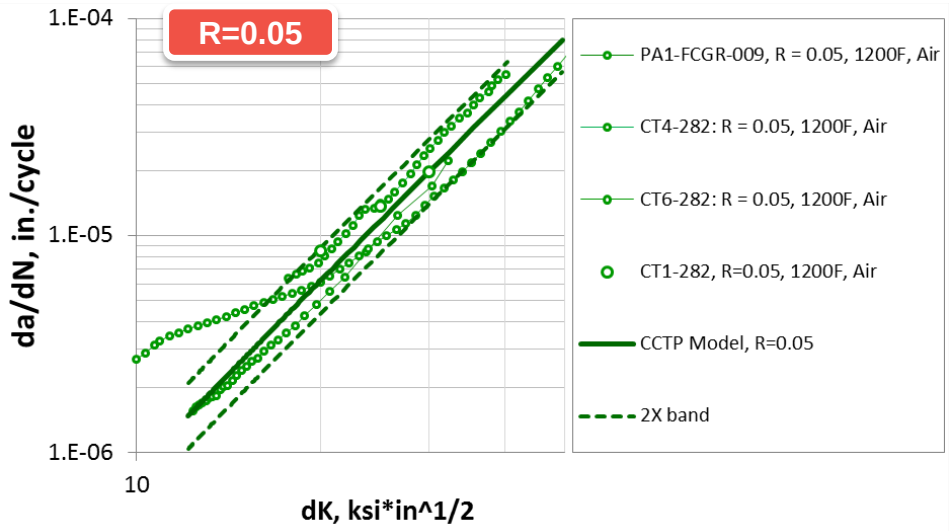
- Predictions at R=0.5
- The shift in curves due to load ratio R predicted by the evolution of crack closure
- Model captures the right trend



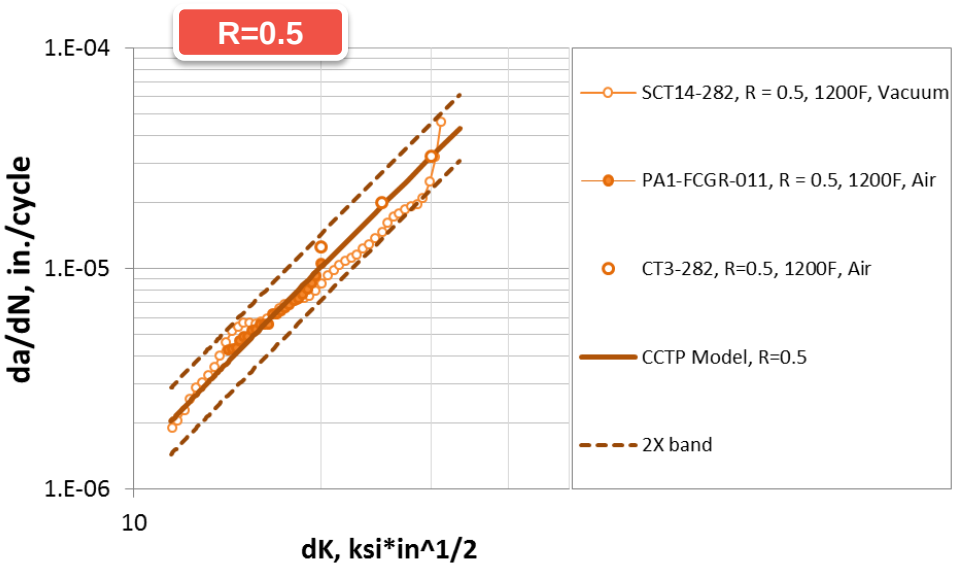
imagination at work

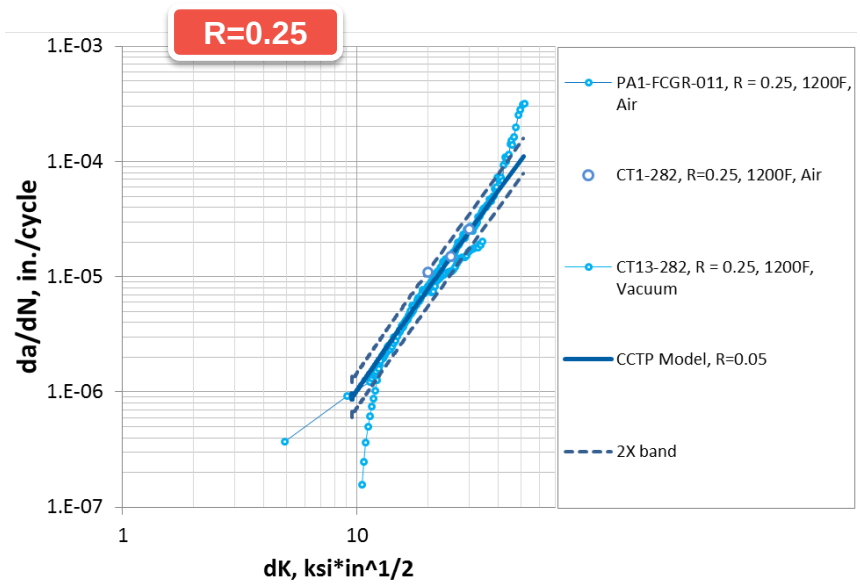
CCTP model predicts both slope and R shift of the da/dN curves

Model prediction at 1200˚F



- Most of the predicted data fall within 2X band, the typical scattering of experimental data
- The data here are tested in vacuum or in air at high cyclic frequency; major environmental damage is the next step





imagination at work

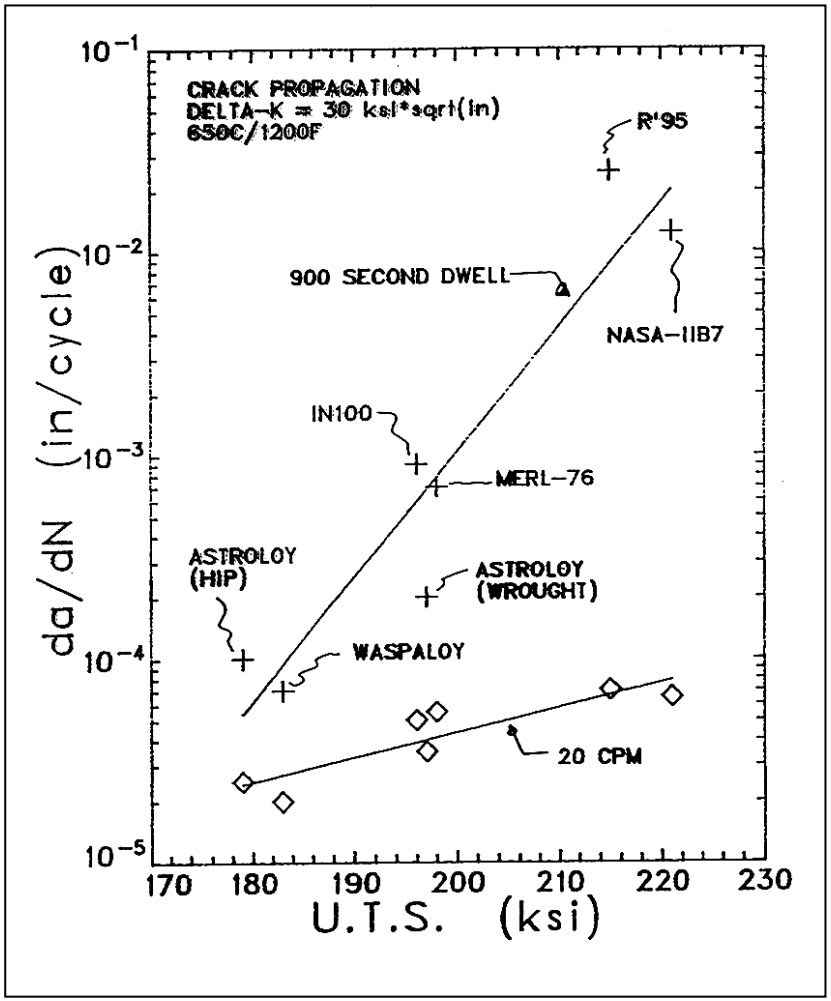
Model predictions capture the average crack growth rates

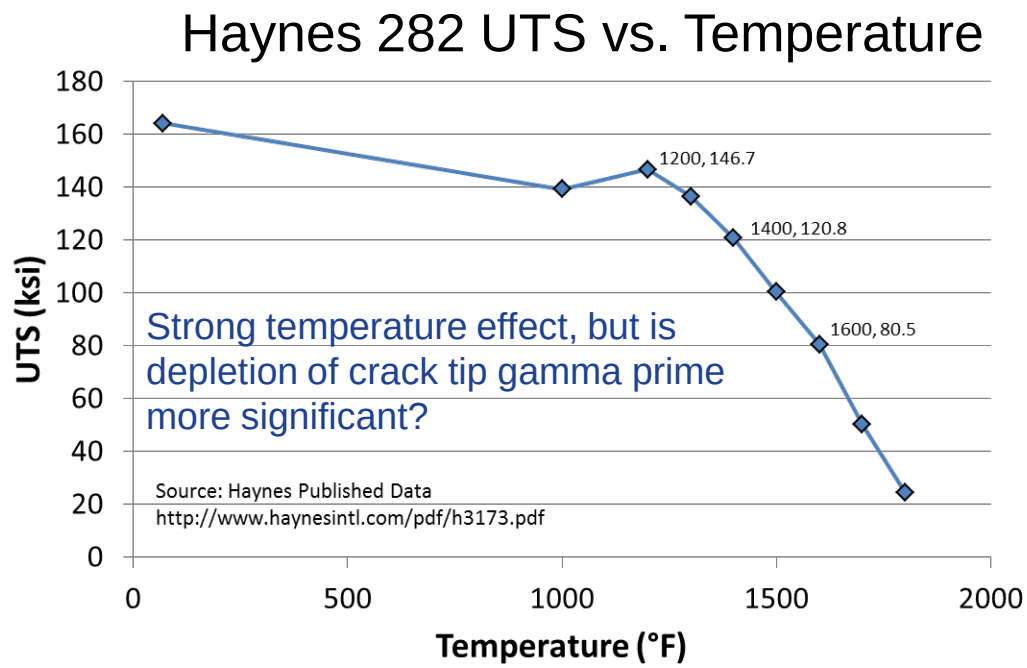
Summary and conclusions

- Environment-fatigue interaction dominates at 1400°F and below; environment-creep-fatigue interaction present at 1600°F
- **1400°F Air**: Ni-Cr-Co-rich spinel formation at crack tip. **1400°F Steam; 1600°F Air and Steam**: Early Al_2O_3 and Cr_2O_3 formation at crack tip and associated gamma prime depletion
- GB-oxygen interaction micromechanism under ab initio study, focusing on oxygen segregation and weakening GB ahead of crack tip
- Mesoscale crack model taking into account GB-O interactions in progress
- Creep strain and rupture predictions agree with experimental data between 1400-1450F, 15-40ksi. Longer time behaviors to be further examined
- Sensitivity of creep to γ' coarsening predicted significant at intermidate stress but negligible below 14ksi (103MPa)
- Multi-scale modeling of fatigue crack integrating confined crack tip plasticity, bulk cyclic behavior, load cycle, hold time and environmental effect, and creep
- Model calibrated at 1200 F and predict for different load (R) ratio; Including crack closure effects predicts the correct dependence on R ratio

Backup slides

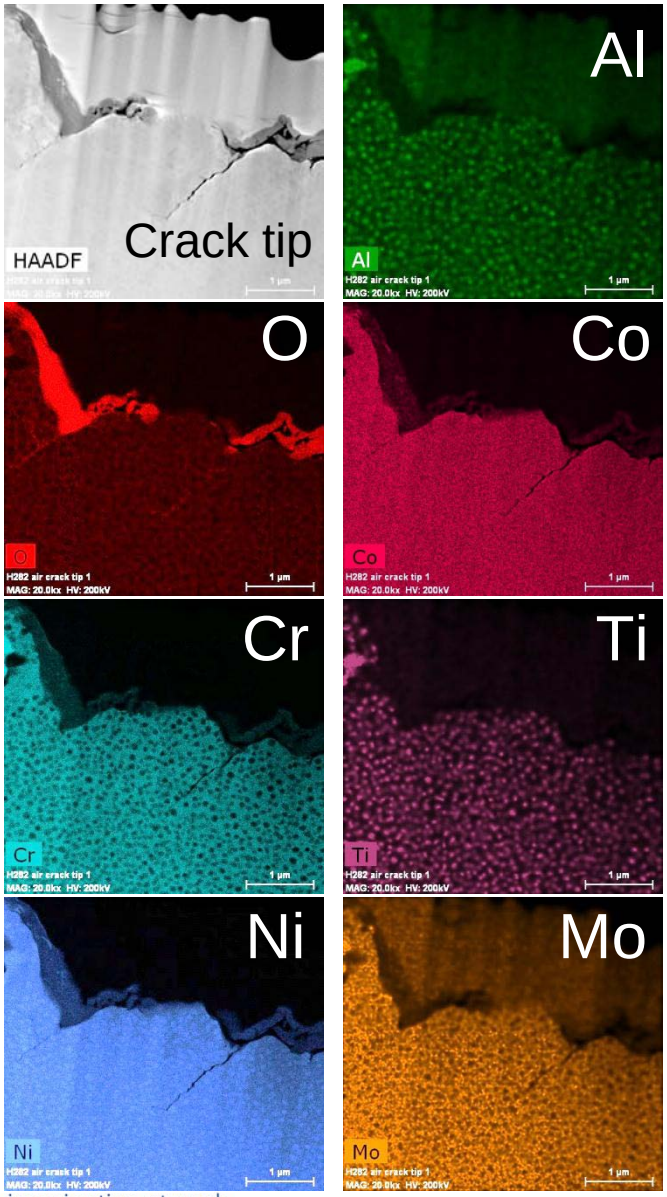
General Effect of Strength on Hold Time Fatigue





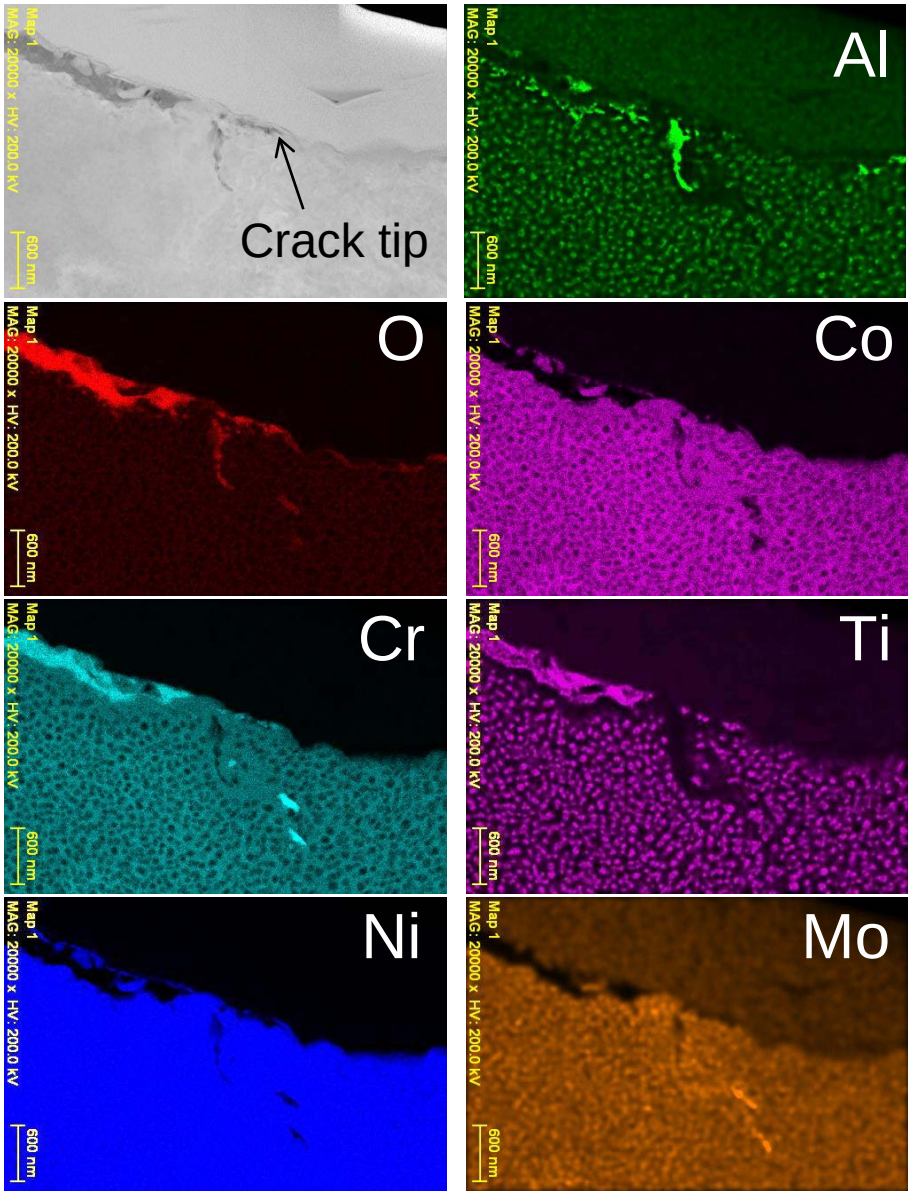
All else fixed, a reduction in strength is *typically* associated with a reduction in hold time crack growth rate

1400°F Air



Crack tip Ni-Cr-Co oxide

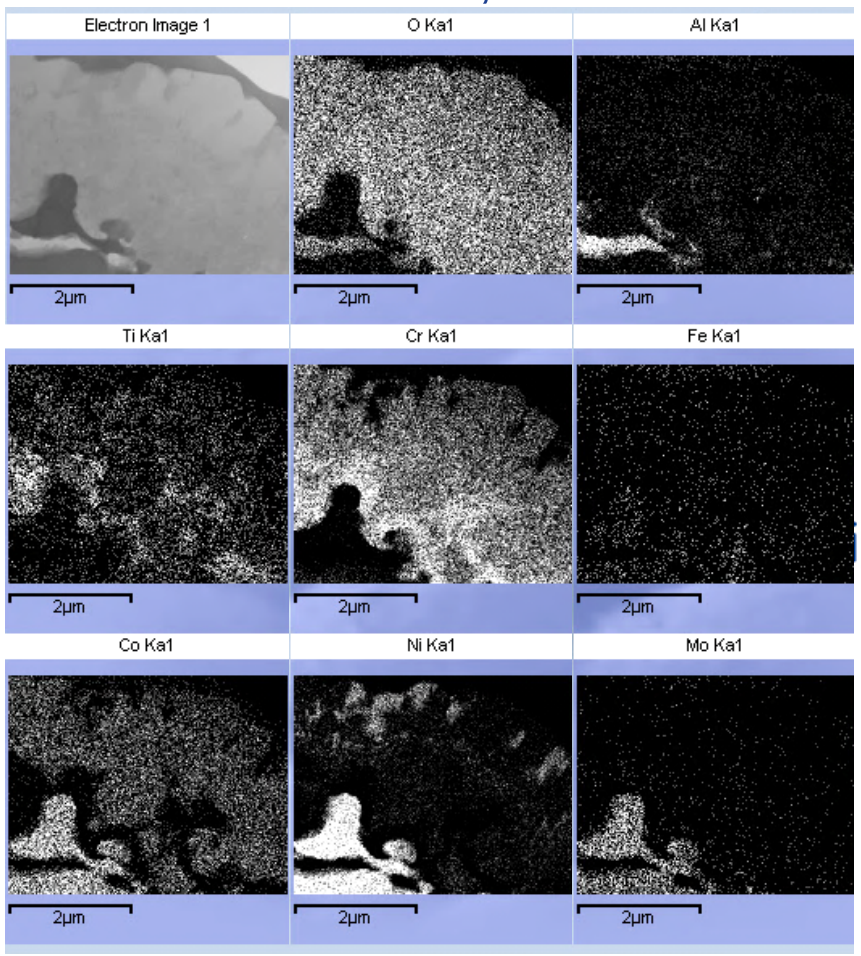
1400°F Steam



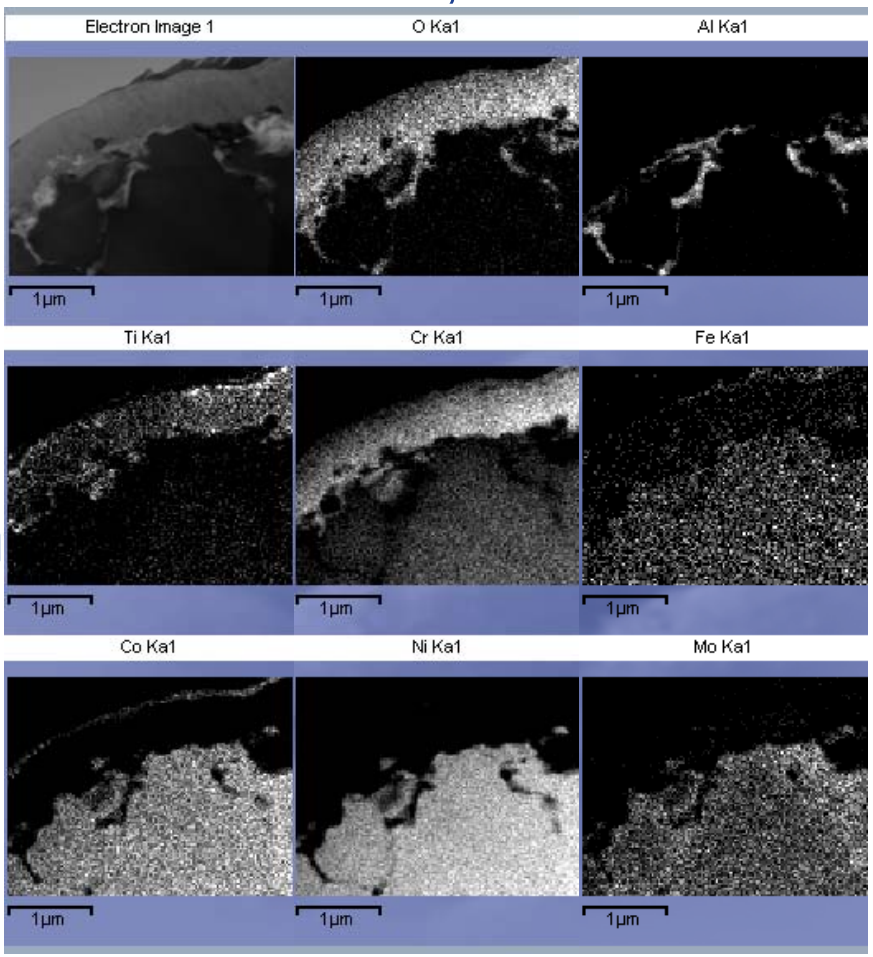
Crack tip Al_2O_3, Ti-O formation; gamma prime depletion

Alloy 282 Elemental Area Maps

1400°F; Air



1400°F; Steam



1400°F Air:

- $Ni(Cr_2O_4)$ spinel
- Relatively uniform Co concentration throughout oxide thickness
- Ti-rich and Cr-rich region within the oxide, directly adjacent to the base metal
- Islands of Ni-O

Common Characteristics:

- Al_2O_3 internal oxidation along grain boundaries

1400°F Steam:

- Bulk of the oxide appears Cr-rich, and diffraction identifies primarily hexagonal Cr_2O_3
- Co-rich layer at the surface of the oxide.
- No evidence of Ni-O

Longer term external surface oxidation

(Essuman e al, 2011)

Steam

Air

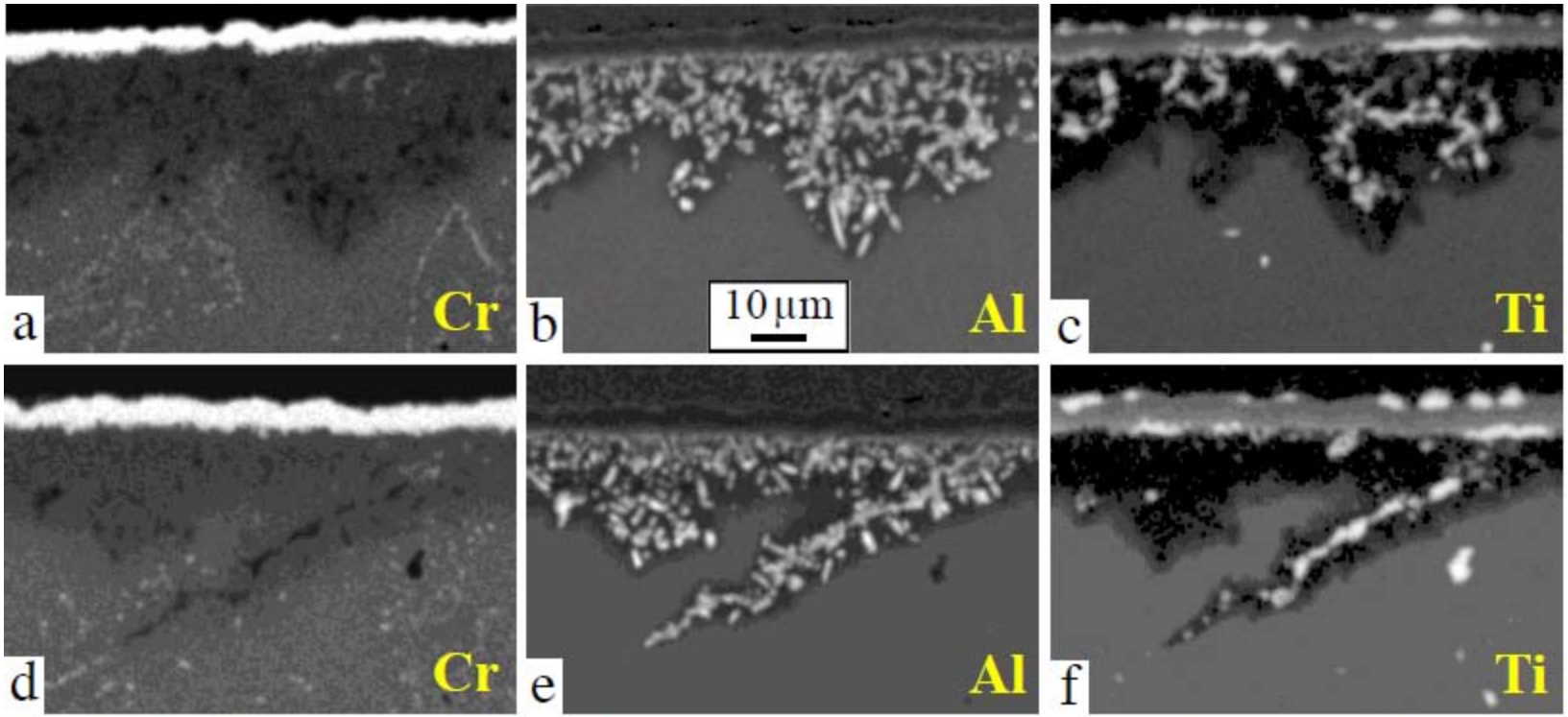
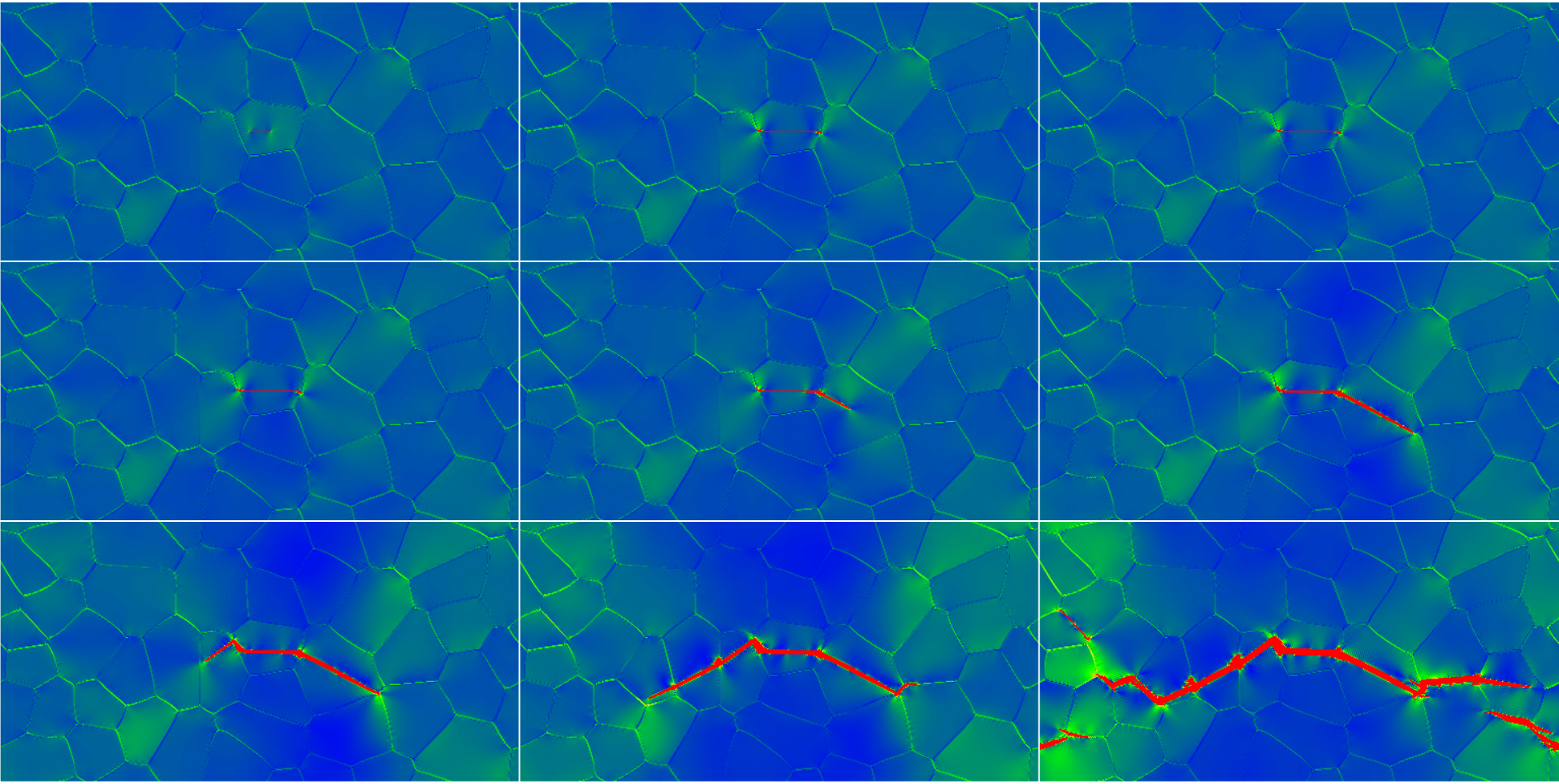


Figure 5. EPMA x-ray maps of the scale formed on equiaxed-grained cast 282 after 5,000h at 800°C (a-c) 17 bar steam and (d-f) 1 bar air; (a,d) Cr, (b,e) Al and (c,f) Ti.

Similar in air & steam

- external scale primarily Cr_2O_3
- internal oxidation a mixture of Al and Ti oxides (more TiO_2 in steam)

Phase field modeling of crack propagation



- Constant static load
- Random grain orientations

Haynes 282 composition and heat treatment

(http://www.haynesintl.com/pdf/h3173.pdf)

Nominal Chemical Composition, Weight %										
Ni	Cr	Co	Mo	Ti	Al	Fe	Mn	Si	C	B
57**	20	10	8.5	2.1	1.5	1.5*	0.3*	0.15*	0.06	0.005

* Maximum ** Nickel as balance

Heat Treatment

HAYNES 282 alloy is provided in the solution-annealed condition, in which it is readily formable. The typical solution annealing temperature is in the range of 2050 to 2100°F (1121 to 1149°C). After component fabrication, a two-step age hardening treatment is required to put the alloy into the high-strength condition. The treatment includes 1850°F (1010°C) / 2 hours / AC (air cool) + 1450°F (788°C) / 8 hours / AC.

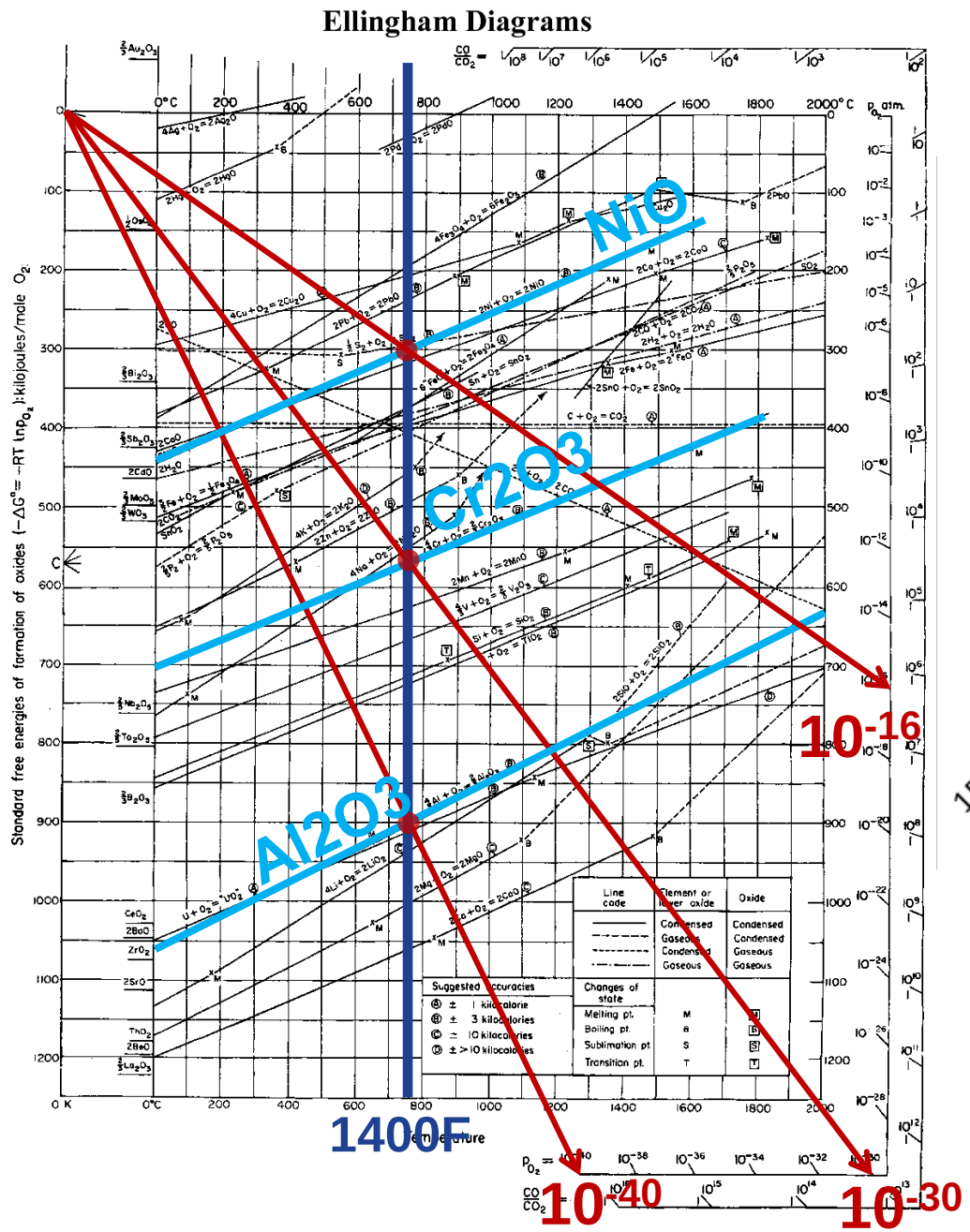
Typical phase composition of oxides

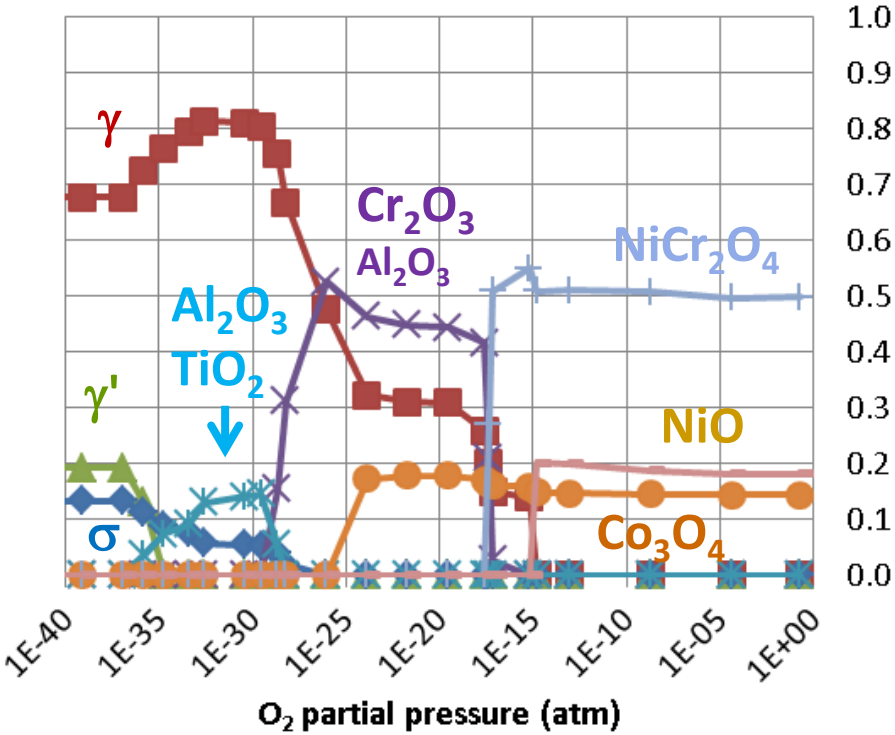
CORUNDUM#1	O	6.00E-01	CR	6.33E-02	FE	2.70E-06			
	AL	3.22E-01	TI	1.48E-02	NI	2.00E-13			
CORUNDUM#2	O	6.00E-01	AL	8.60E-02	FE	2.74E-06			
	CR	2.44E-01	TI	7.00E-02	NI	2.00E-13			
SPINEL#1	O	5.25E-01	FE	6.23E-02	AL	3.94E-13			
	CO	3.94E-01	CR	1.88E-02	NI	3.94E-13			
SPINEL#2	O	5.71E-01	NI	1.43E-01	FE	2.82E-06			
	CR	2.51E-01	AL	3.47E-02	CO	8.57E-13			

IONIC_LIQ

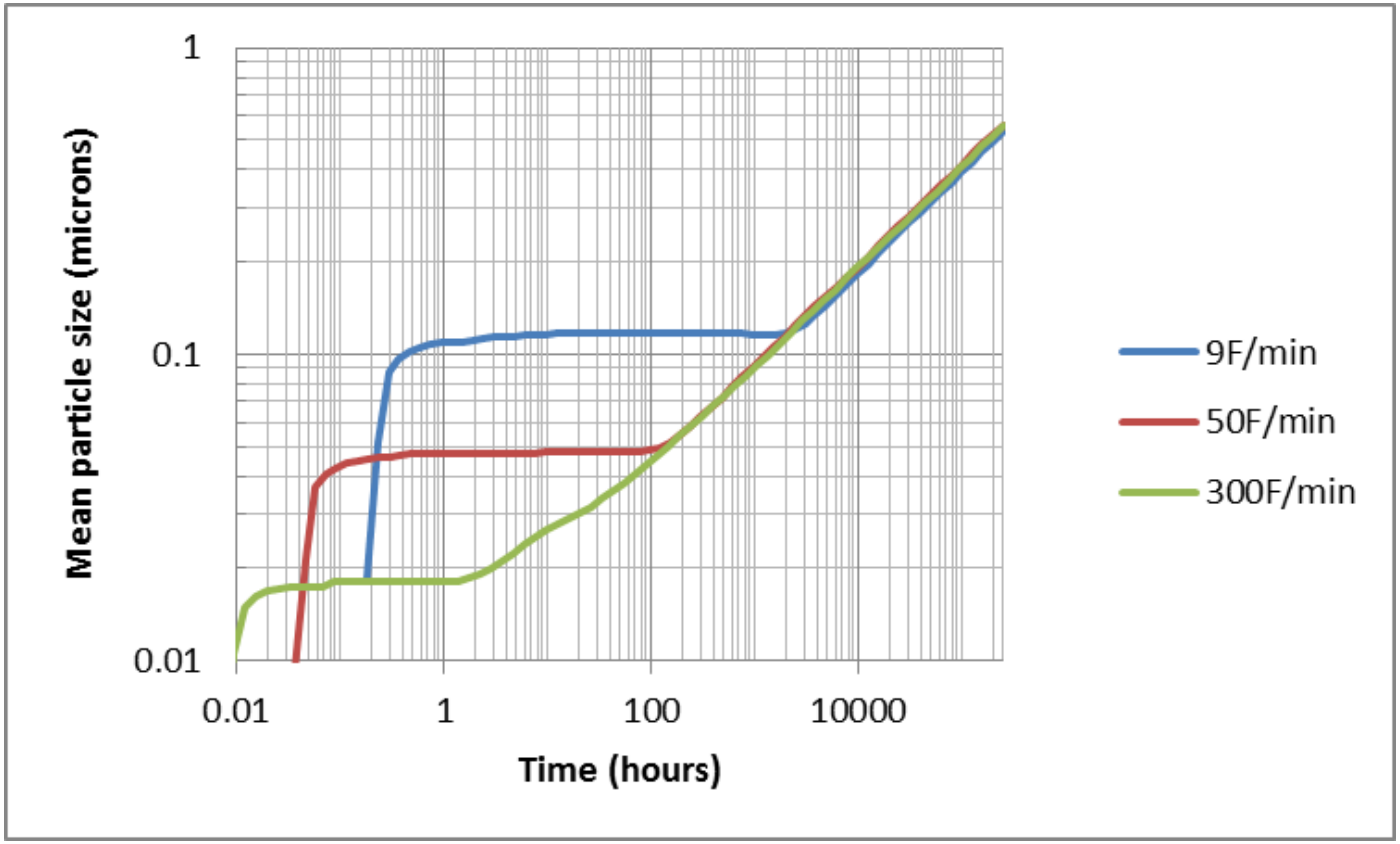
O 5.02161E-01 NI 2.16939E-01 CO 2.15164E-04 AL 1.24565E-06
TI 2.51078E-01 MO 2.95961E-02 FE 7.67877E-06 CR 9.32971E-07
Sublattice 1, Number of sites 1.1102E+00
NI+2 8.79155E-01 FE+2 3.11184E-05 TI+2 1.00000E-12
MO+4 1.19939E-01 CR+2 2.97972E-06
CO+2 8.71961E-04 AL+3 1.00000E-12
Sublattice 2, Number of sites 2.2399E+00
TIO2 5.04337E-01 ALO2-1 2.50211E-06 FEO3/2 5.54747E-11
VA 4.95655E-01 CRO3/2 3.97111E-07 COO3/2 1.00000E-12
O-2 5.05161E-06 MOO3 2.72860E-09

Intersection is equilibrium point:
Oxide forms at P(O2) higher than this point.



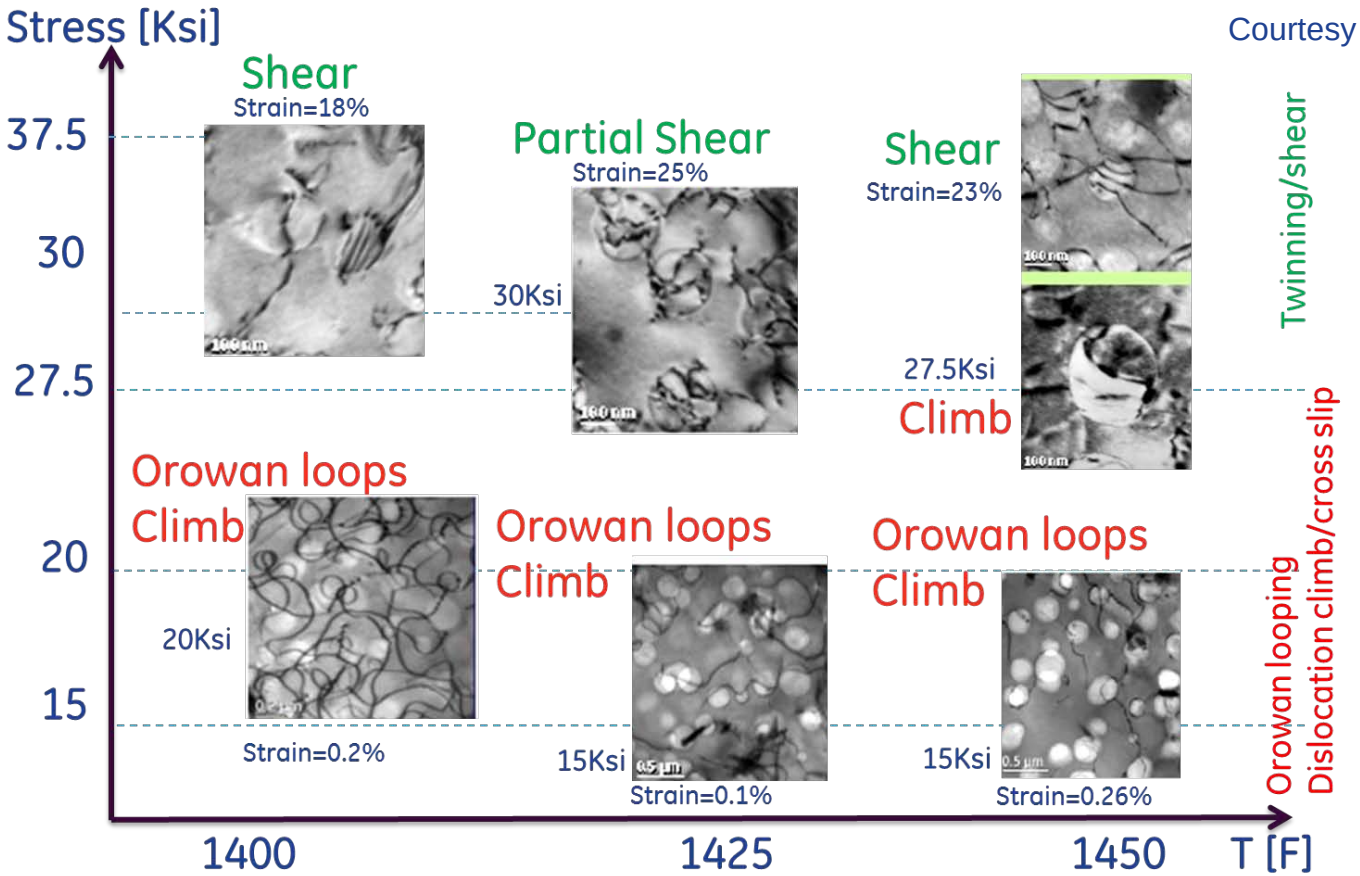


Predicted γ' coarsening at 1400˚F for Alloy 282



Alloy 282 creep mechanism understanding (Task 5)

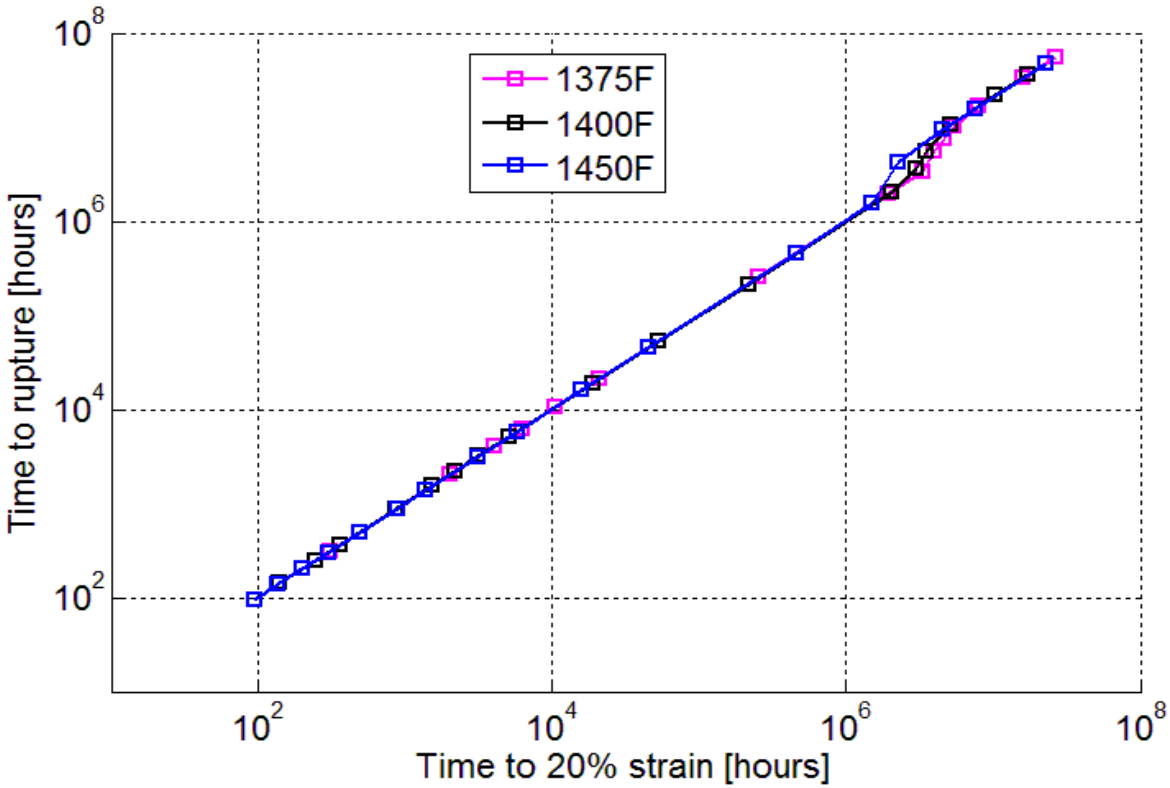
Courtesy M Karadge



- Low stress: dislocation looping & climb,
- Higher stress: γ' shearing
- Microtwinning at very low stress, low temperature

Dislocation climb-bypass is the main observation at low stresses

Time to rupture is very close to time to 20% strain



Summary and Plans

1. **Scatter in FCGR data**
   - 2x scatter is typically observed in FCGR measurements
   - The expectation from the model is to be able to predict average behavior
2. **Time dependent description of fatigue crack growth** $\frac{da}{dt} = \alpha \left|\frac{d\rho}{dt}\right|$
   - Proposed procedure is time based, which is a switch from classical fracture mechanics approach (Paris law, cycle based)
   - Time based models make it more convenient to incorporate other time dependent damage mechanisms contributing to crack growth (such as oxidation and creep)
3. **Model prediction and data at 1400F**
   - The CCTP model will need to be calibrated and validated at 1400F, where environment effect is more prominent
   - More specimens are in queue to capture FCGR response under complex missions and harsh environment at 1400F; the collected data will be used for validation purposes
4. **Model extension to account for creep-environment effect** $\frac{da}{dt} = \alpha \left|\frac{d\rho}{dt}\right| + \frac{\partial a}{\partial t}_{creep} + \frac{\partial a}{\partial t}_{oxidation}$
   - A common modeling framework is proposed to capture oxidation-corrosion effect through a set of differential equations
   - Approach to include creep effect is currently being investigated, although, at 1400F, creep deformation does not seem to be a dominant damage mechanism