



Grain Boundary Character and Creep-Fatigue Crack Tip Kinetics

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High Temperature Materials: Importance

- Applications:

- Aircraft Engines
- Rocket Engines
- Power Systems
- Automotive Systems



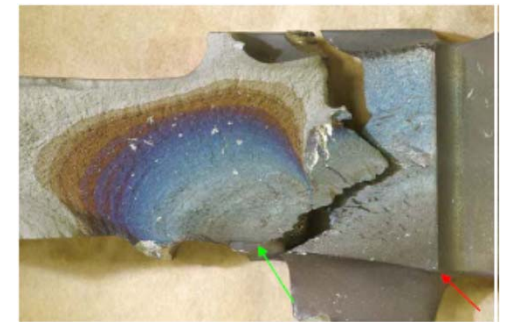
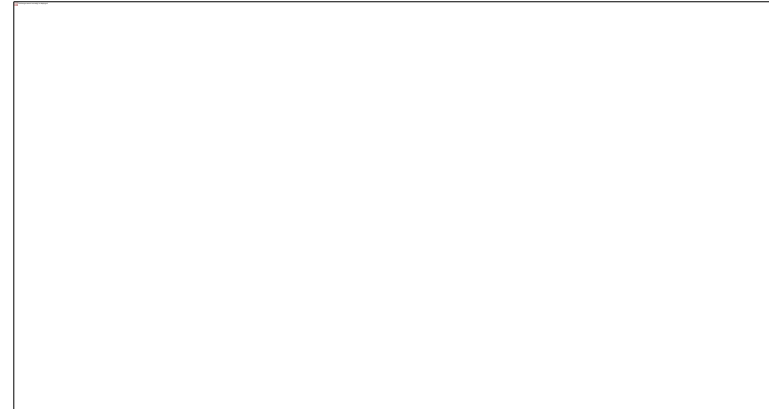
- Goal: To understand the fundamental mechanisms of failure due to fatigue, fracture, and corrosion and develop lifetime prediction models.
- Mechanical behavior and lifetime prediction critical for:
 - Safety
 - Economics

Motivation

2006 LAX Failure

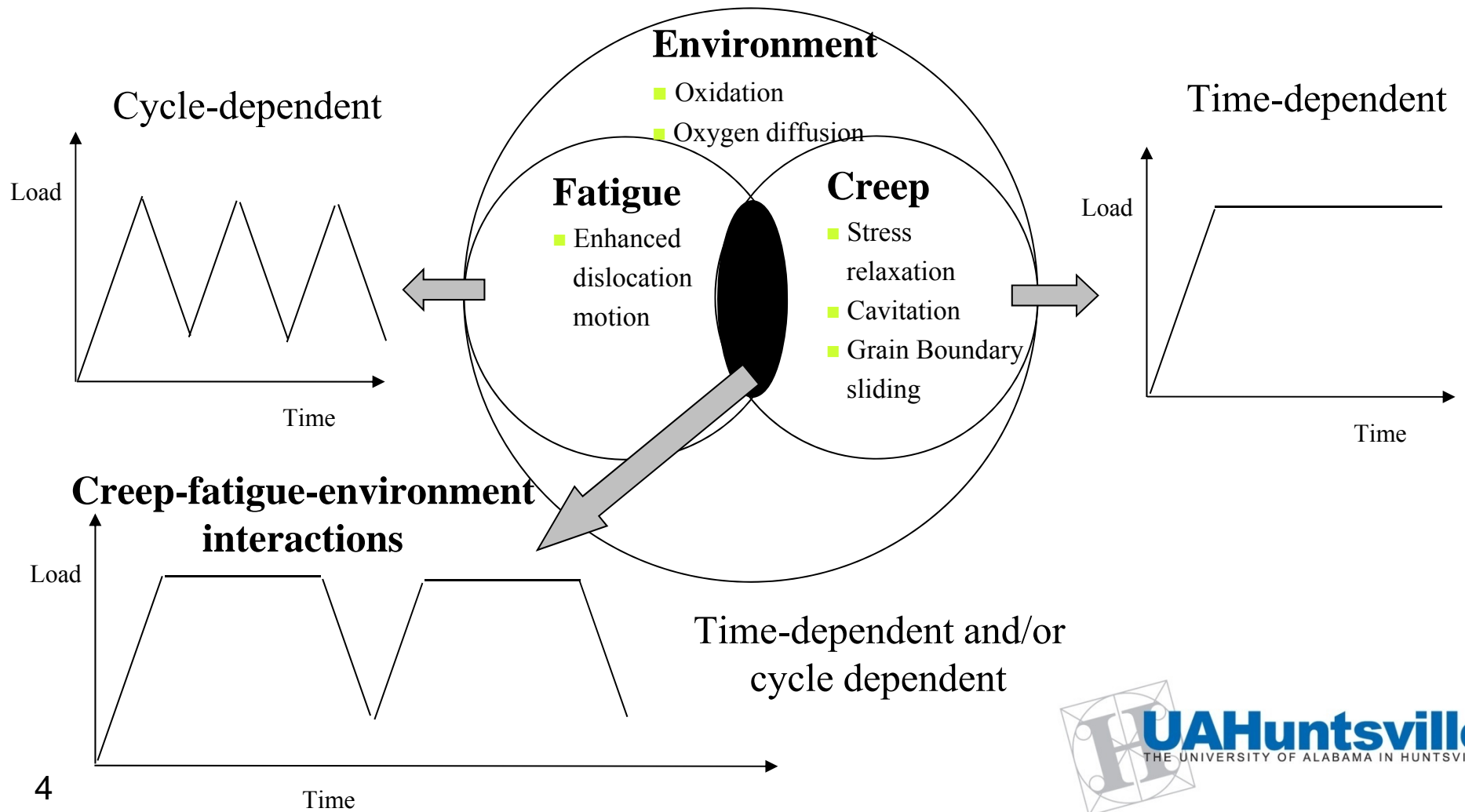


2002 Brisbane Failure



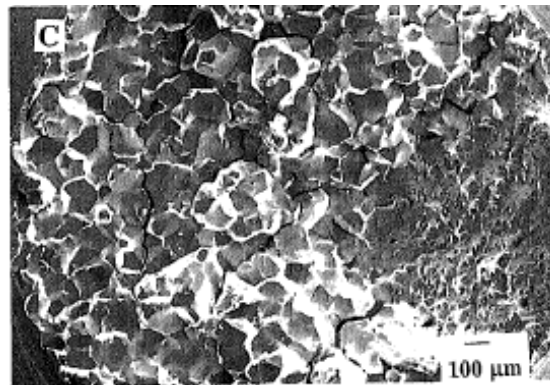
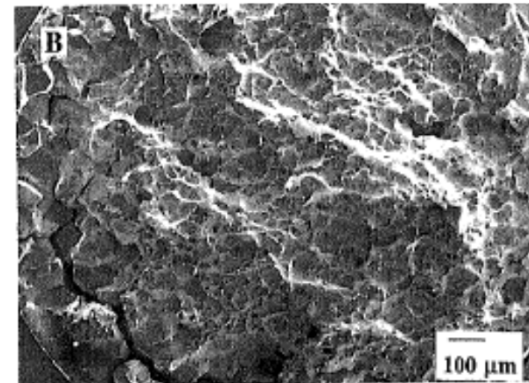
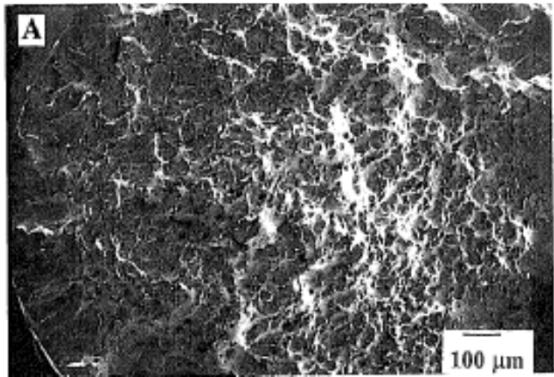
Elevated Temperature Fatigue Crack Growth

Comprehensive Approach



Fracture Mechanisms

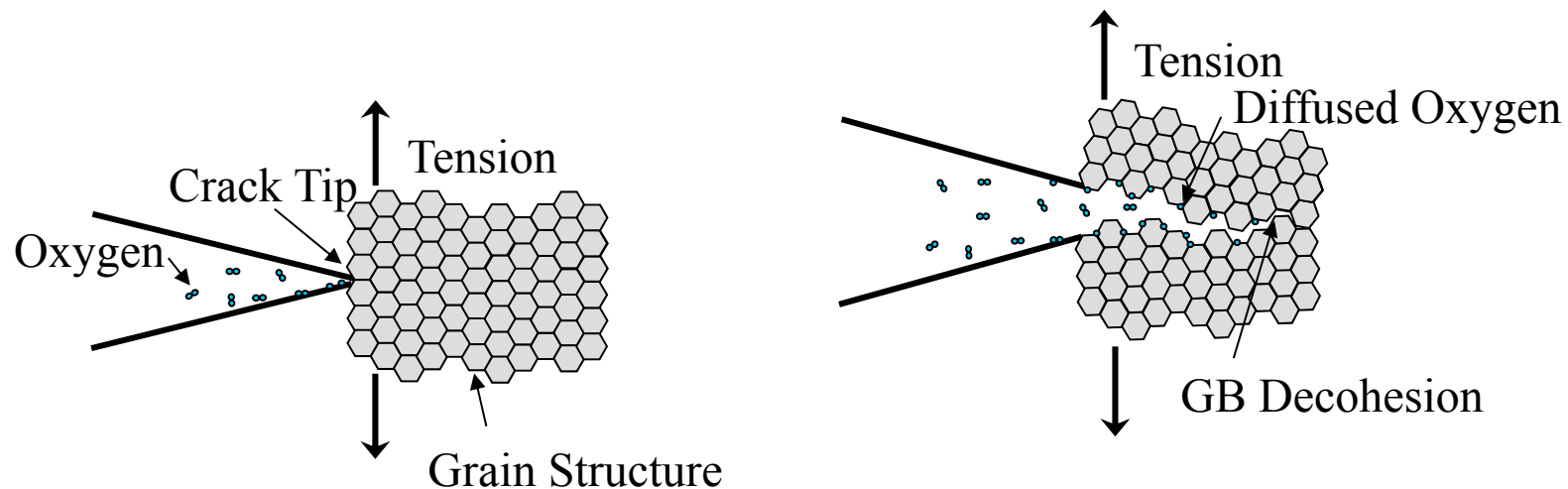
An oxygen partial pressure threshold has been observed for the transition from transgranular to intergranular fracture .



Fracture surfaces corresponding to different oxygen partial pressures A, 10⁻⁴ Torr; B, 1 Torr; C, 4 Torr (from Andrieu, et al., 1992.)

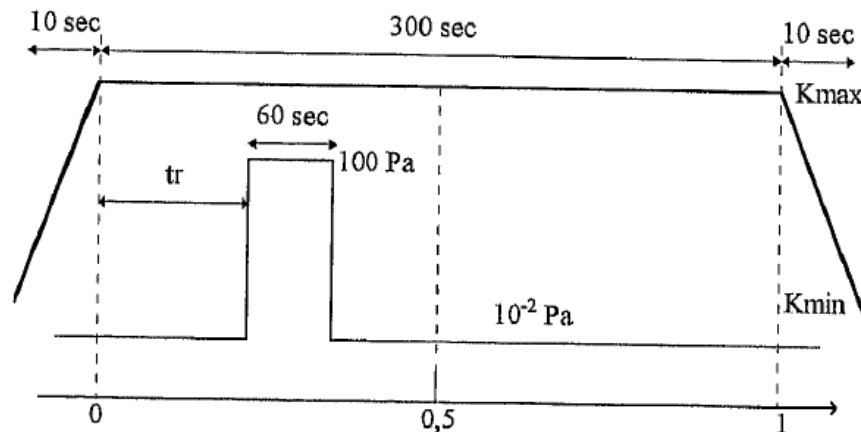
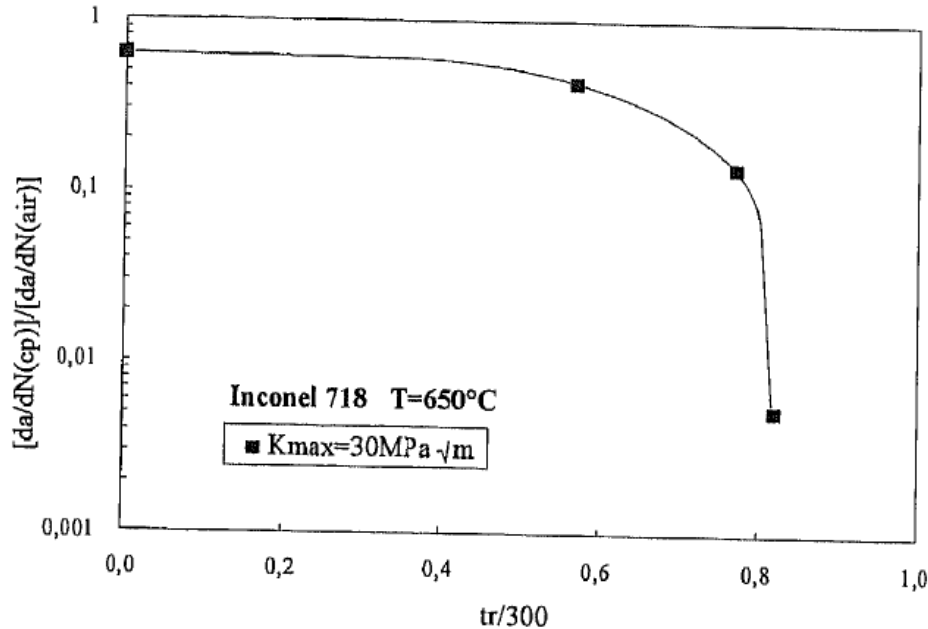
Possible Embrittlement Steps

- Temperature is elevated and load is applied
- Oxygen diffuses through air to the crack tip
- Oxygen adsorbs and dissociates on the crack surface and forms an oxide
- Oxygen diffuses along grain boundaries ahead of the crack tip
- Oxide forms on grain boundaries and reduces their cohesive strength
- Elevated temperature causes creep/stress relaxation and reduces driving force for grain boundary diffusion



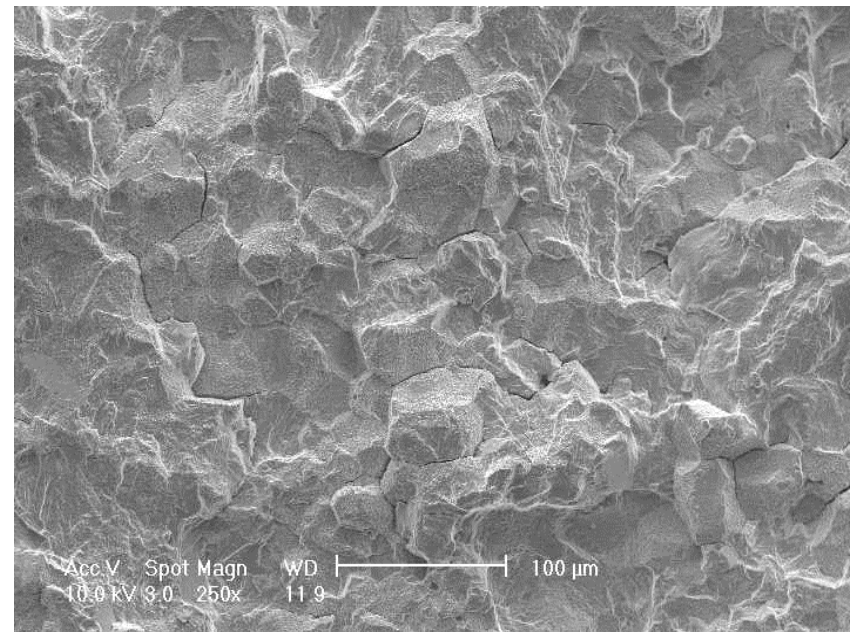
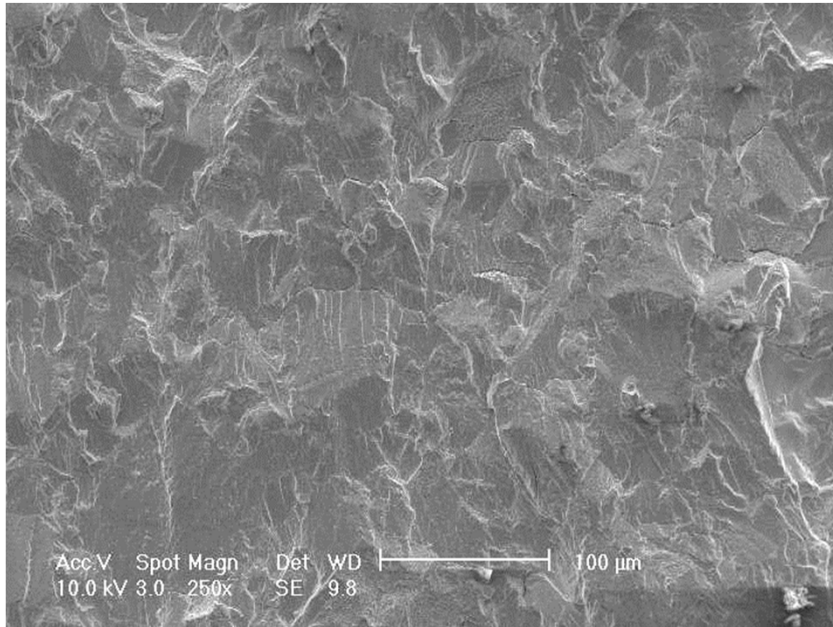
Rate controlling step must be identified

Influence of Stress Relaxation

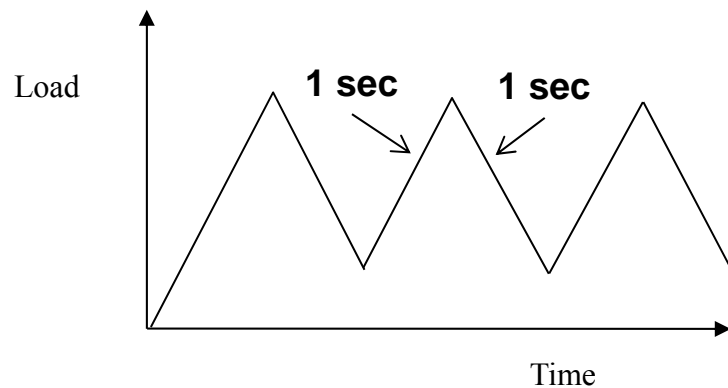


- Oxygen pressure pulse at different locations during the hold period
- “The detrimental interaction between oxygen and local mechanics is efficient during the first 200 seconds of the hold time”
- Once the crack tip stresses have relaxed, oxygen has limited influence

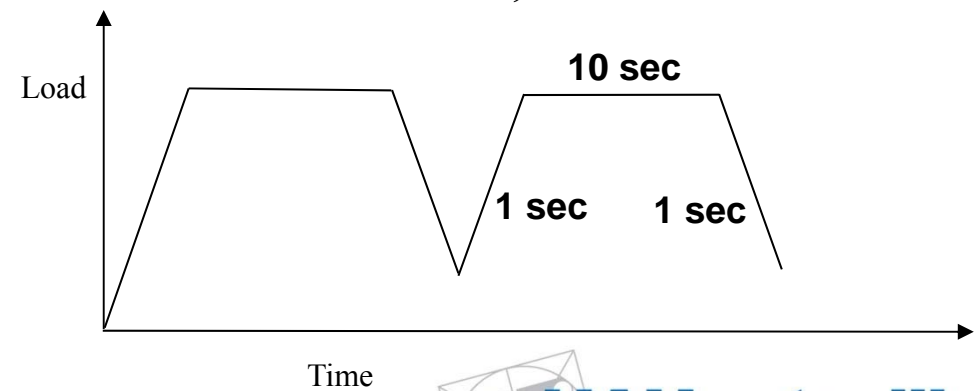
Fracture Surface Analysis: ME3, Air, 704°C



0 sec hold time, $\sim\Delta K=30\text{MPa m}^{1/2}$



10 sec hold time, $\sim\Delta K=30\text{MPa m}^{1/2}$



We need to understand the crack tip kinetics

Activation Energies

Kinetic Process	Q (kJ/mol)	Temp Range (°C)	Source
Stress relaxation of 718	332.9	700-1000	Zhou et al., 2011
Diffusion of oxygen along particle interface in Ni (used to approximate rate along grain boundaries)	300.9	800-1100	Stott, 1984
Diffusion of Ni in Fe-55Ni-19Cr	299.0	1026-1296	Ruzickova, 1988
Reaction of NiO	220.9	900-1300	Rosa, 1982
Reaction of TiO ₂	167.0	600-800	Gomes, 1979
Diffusion of oxygen in Ni	164.0	850-1400	Park and Alt., 1987
Grain boundary creep	~150	~750-950	Starink and Reed, 2008

- As stated by Tang and Plumtree (1991), if the crack tip atomic bonds are strained to their theoretical strength, then the activation energy at the crack tip becomes,

$$Q_t = (0.35 - 0.71)Q_o$$

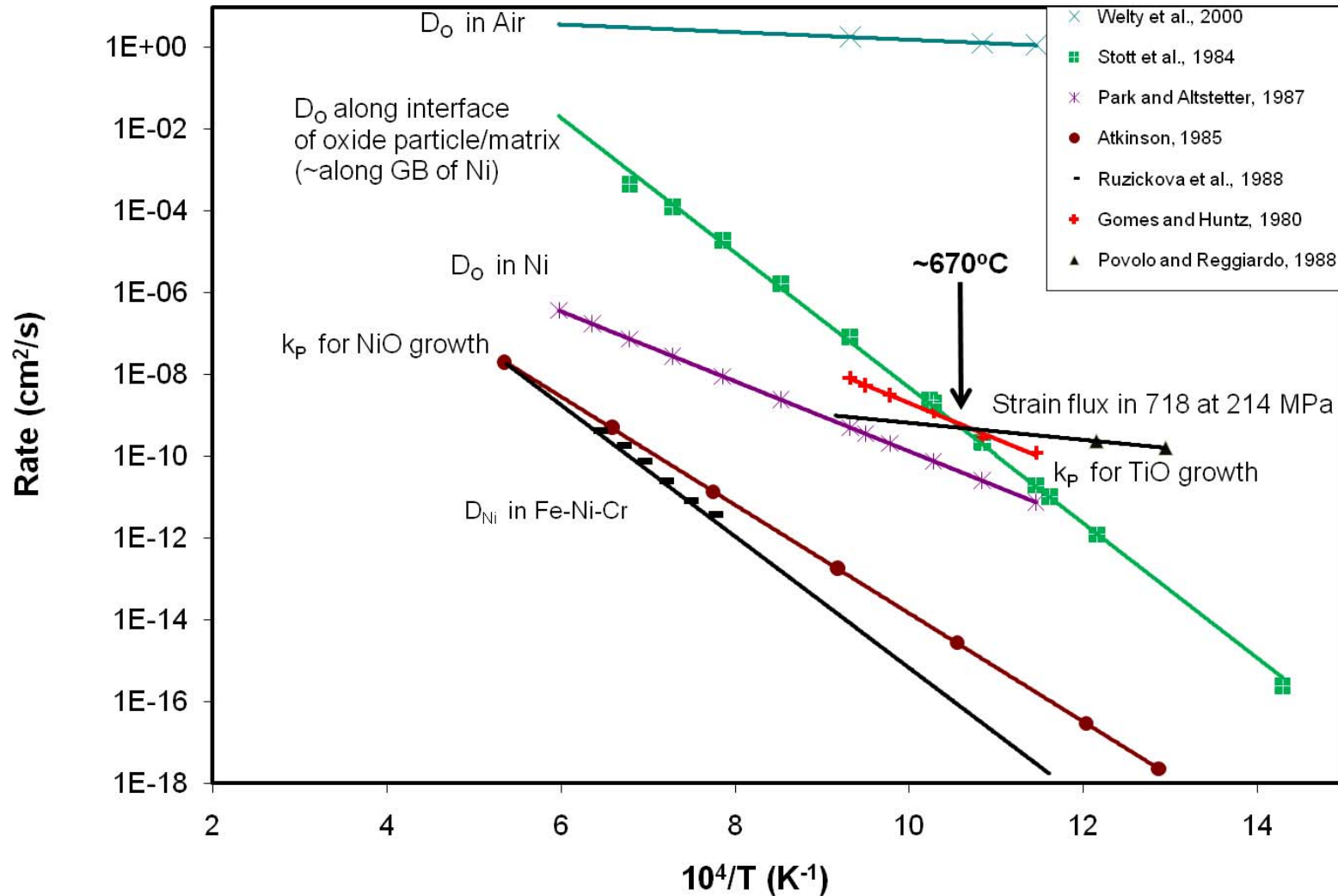
- Grain boundary creep, oxygen diffusion, and titanium oxide formation have similar activation energies
- What if they are all active?
- We need to compare the rates for each process

Comparison of the Kinetics

The processes:

- Diffusion rate of oxygen in air
- Diffusion rate of oxygen in nickel
- Diffusion rate of oxygen along grain boundaries
- Diffusion rate of nickel through an Fe-Ni-Cr alloy
- Rate of formation of NiO and TiO₂
- Creep flux for the Ni-base superalloy 718
 - Determined using strain rate versus temperature data
 - Assumed a 12.7mm standard cylindrical sample
 - Proportional to stress relaxation at the crack tip

Kinetic Chart



Evans, J.L., "Method for Comparing the Crack Tip Kinetics During Creep-Fatigue Loading of Nickel-Base Superalloys," Materials Science and Engineering A, Volume 528, Number 15, June 15, 2011, pp. 5306-5308.

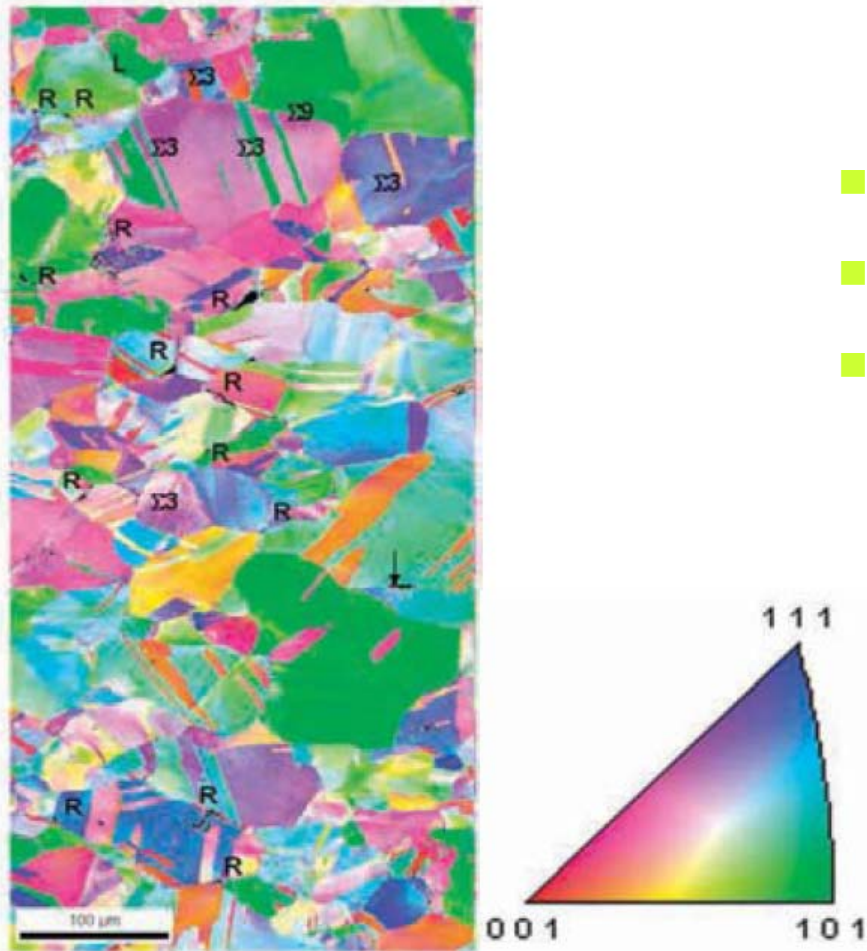


Facilities

- MTS 22 kip servohydraulic test system
- Satec 120 kip electromechanical test system
- 1.2 kW Ameritherm induction heater for mechanical property tests
- ATS furnace (1000°C) for mechanical tests
- Tube furnace (1200°C) for oxidation studies
- Vacuum furnace for use in mechanical tests
- 2-D Correlated Solutions Digital Image Correlation System for crack growth measurements



Grain Boundary Character

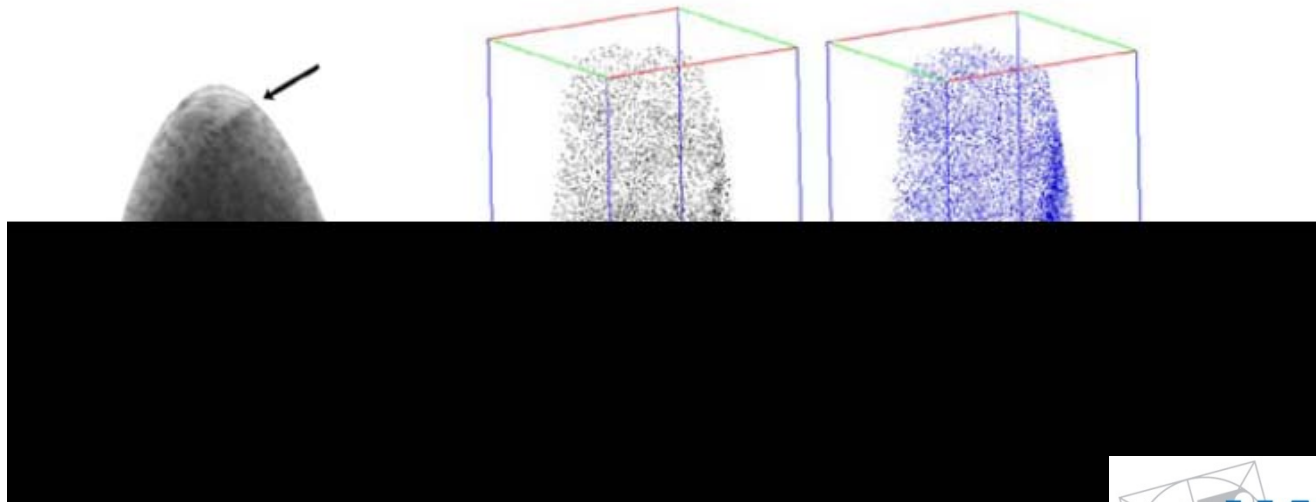


- Electron Backscatter Diffraction
- Determine Grain Orientation
- Special grain boundaries exist when a high fraction of coincident site lattice and twin boundaries are present

[Boehlert et al., 2008]

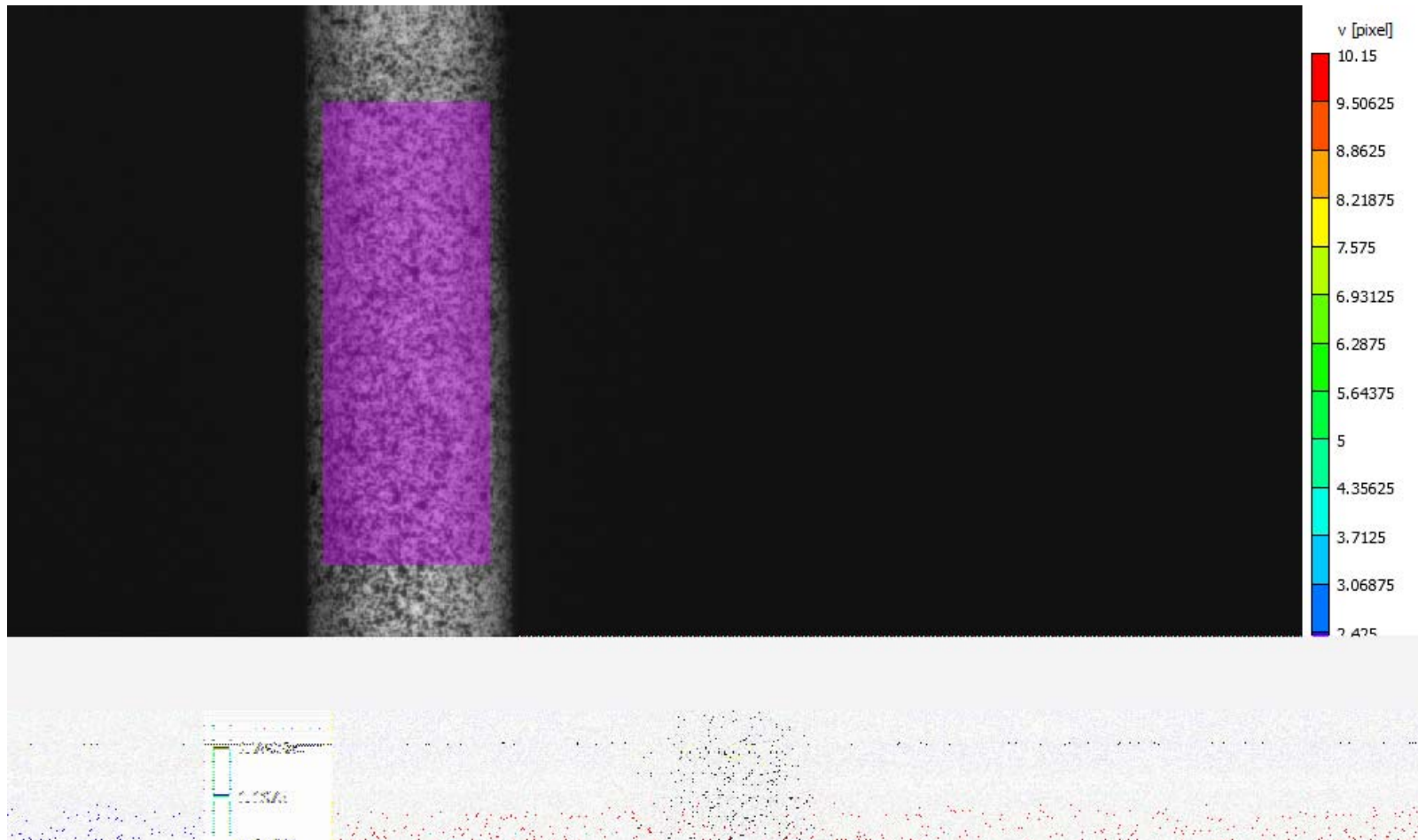
Atom Probe Tomography

- Atomistic chemistry can be determined
- 3-D reconstruction of the chemical distributions of the sample
- Grain boundaries will be investigated to understand the oxidation behavior



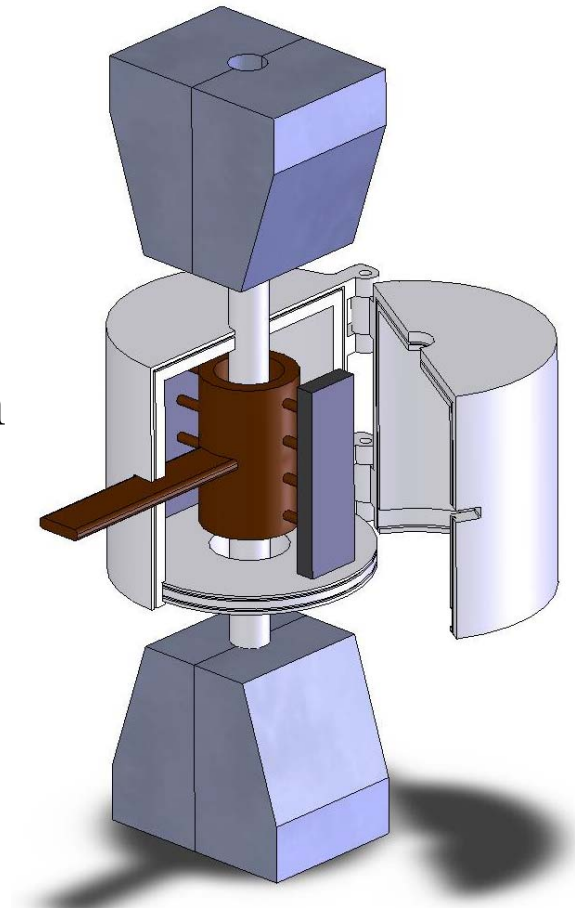
[Viskari and Stiller, 2011]

Digital Image Correlation



Proposed Future Work

- Investigate the environmental effects on elevated temperature fatigue of nickel and nickel alloys (DOE BES)
- Fatigue behavior of future turbine materials in steam (GE, Siemens, DOE, others)
- 3-D Crack growth reconstruction using a laboratory X-ray source [with UCSF] (NSF, DOE, NIH)
- Laser-assisted Machining of Titanium (AAR Precision)
- Fatigue of MEMS Devices [with John Williams] (NSF)



Summary

- High temperature fatigue is an important engineering and scientific problem
- A number of time-dependent processes are potentially operational during high temperature hold periods
- A chart has been proposed that compares the kinetics of the various processes at the crack tip including the rates of diffusion of oxygen, rate of diffusion of nickel through an Fe-Ni-Cr alloy, the reaction rate of NiO, and a creep flux.
- Grain boundary character can influence this behavior
- High Temperature test capability with Digital Image Correlation along with advanced characterization techniques (EBSD, Atom Probe Tomography) are being employed

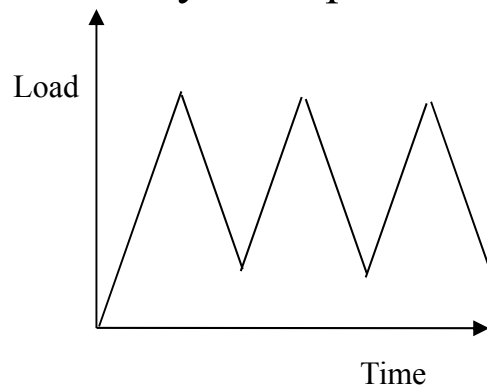


Crack Growth Model

- This method was first proposed for modeling a corrosion-fatigue process [Wei and Landes, 1969]
- It was later also applied to the creep-fatigue process in the following form [Wei and Huang, 2002]

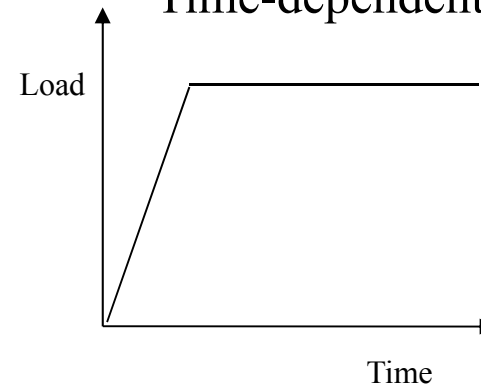
$$\left(\frac{da}{dN}\right)_{tot} = \left(\frac{da}{dN}\right)_{cyc} + \left(\frac{da}{dN}\right)_{td}$$

Cycle-dependent

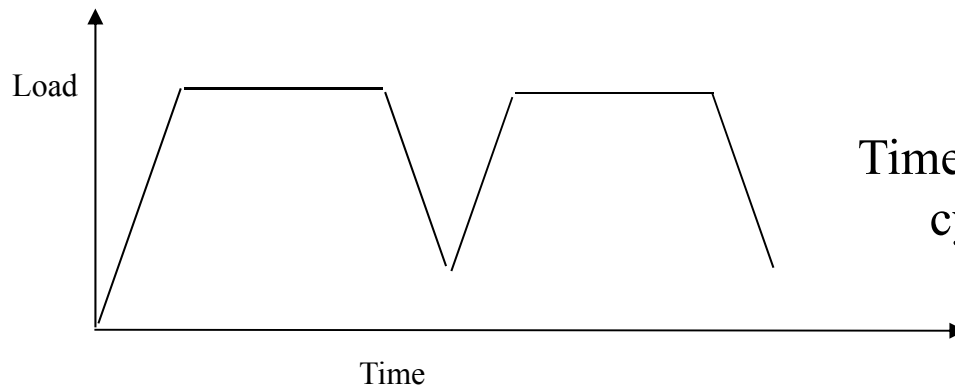


+

Time-dependent



=



Time-dependent and/or
cycle dependent

Cycle-Dependent Components

$$\left(\frac{da}{dN}\right)_{cyc} = \left(\frac{da}{dN}\right)_{ath} + \left(\frac{da}{dN}\right)_{dl}$$

$$\left(\frac{da}{dN}\right)_{ath} = q \Delta K^{n_1}$$

$$\left(\frac{da}{dN}\right)_{dl} = c_0 \cdot \Delta K^{m_0 + \frac{c_1}{RT}} \cdot \exp\left(-\frac{Q_0}{R_G T}\right) \quad (\text{Yoon et al., 2006})$$

- Based on thermal activation of dislocations
- Crack growth is a function of the activation energy for dislocation motion

Time-Dependent Component

$$\left(\frac{da}{dN}\right)_{td} = \int_0^{t_h} \frac{da}{dt} dt$$

da/dt is needed – incorporates environment and temperature (Used Liu, 1970 Methodology)

$$\mathbf{J} = -D \left(\nabla C + \frac{C}{kT} \nabla U \right)$$

Flux of oxygen under a stress gradient
(Shewmon, *Diffusion in Solids*, 1963)

$$C = C_0 \exp\left(-\frac{U}{kT}\right)$$

Concentration as a function of stress potential

$$U = p\Delta V$$

$$p = -\frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$$

Hydrostatic stress at crack tip

$$\Delta V = 4\pi\gamma^3$$

Volume change around diffusing atom

Time-Dependent Component

$$\sigma_{ij} = \left[\frac{K^2(1-\nu^2)}{EI_n A(n+1)tr} \right]^{\frac{1}{n+1}} \hat{\sigma}_{ij}(\theta, n) \quad \text{Crack tip stress field eqns – small-scale creep}$$

$$C = C_0 \exp \left(\frac{4\pi\gamma^3}{3kT} \left[\frac{K^2}{tr} \right]^{\frac{1}{n+1}} \beta (\hat{\sigma}_{xx}(\theta, n) + \hat{\sigma}_{yy}(\theta, n)) \right) \quad \text{Insert stress field equations into concentration equation}$$

$$\beta = (\nu + 1) \left[\frac{(1-\nu^2)}{EI_n A(n+1)} \right]^{\frac{1}{n+1}}$$

$$-\frac{\partial C}{\partial t} = kC$$

Assume oxygen reacts along grain boundaries according to a first order reaction rate

$$k = \bar{A} \exp \left(-\frac{Q}{RT} \right)$$



Time-Dependent Component

$$\frac{da}{dt} = -\alpha \frac{\partial C}{\partial t} \quad \text{Assume crack growth rate is proportional to reaction rate}$$

$$\frac{da}{dt} = \alpha \bar{A} \exp\left(-\frac{Q}{RT}\right) C_0 \exp\left(\frac{4\pi\gamma^3}{3kT} \left[\frac{K^2}{tr}\right]^{n+1} \beta(\hat{\sigma}_{xx}(\theta, n) + \hat{\sigma}_{yy}(\theta, n))\right)$$

$$\frac{da}{dt} = A' \exp\left(\Psi K^{\frac{2}{1+n}}\right)$$

$$\Psi = \Psi' \left(\frac{1}{T}\right) \left(\frac{1}{t}\right)^{\frac{1}{n+1}}$$

$$A' = A'' \exp\left(-\frac{Q}{R_G T}\right)$$

Comprehensive Crack Growth Model

$$\left(\frac{da}{dN}\right)_{tot} = \left(\frac{da}{dN}\right)_{cyc} + \left(\frac{da}{dN}\right)_{td}$$

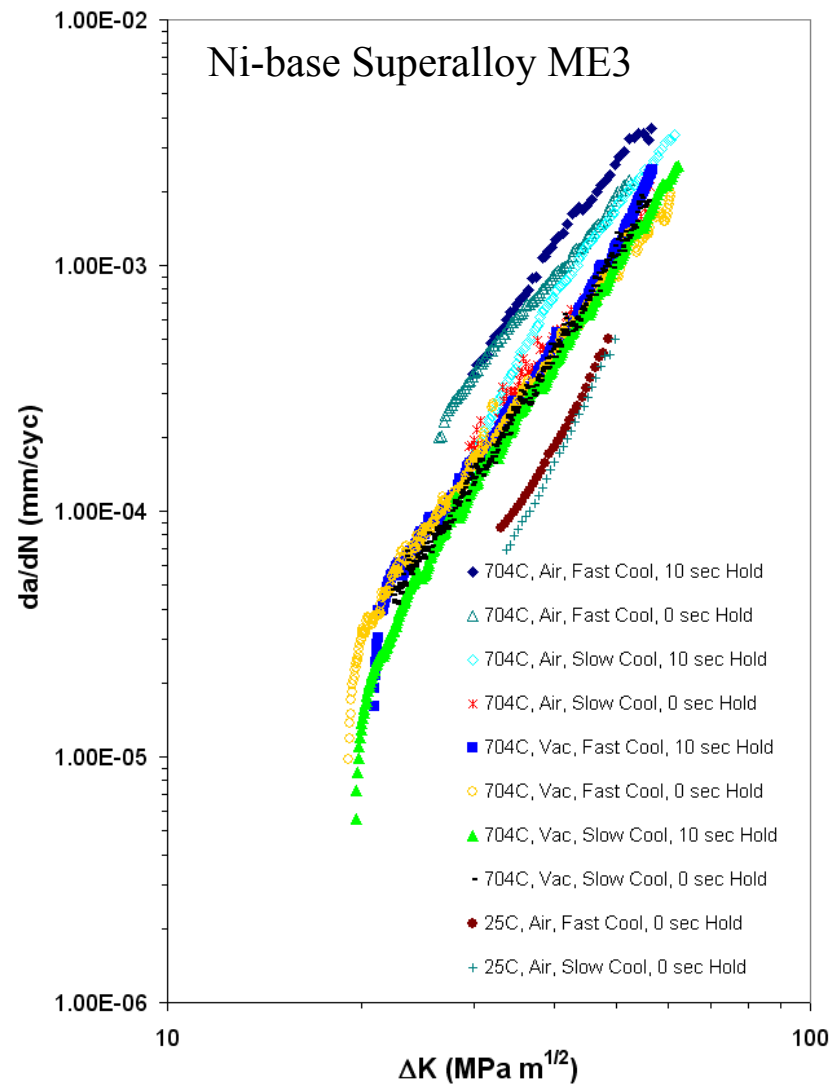
$$\left(\frac{da}{dN}\right)_{tot} = q\Delta K^{n_1} + c_0 \cdot \Delta K^{m_0 + \frac{c_1}{RT}} \cdot \exp\left(-\frac{Q_0}{R_G T}\right) + \int_0^{t_h} A'' \exp\left(-\frac{Q}{R_G T}\right) \exp\left(\Psi' \left(\frac{1}{T}\right) \left(\frac{1}{t}\right)^{\frac{1}{n+1}} \left(\frac{\Delta K}{1-R}\right)^{\frac{2}{n+1}}\right) dt$$

- Comprehensive model has cycle-dependent and time-dependent components
- Includes creep, environment, and athermal and thermally activated fatigue

Evans, J.L. and Saxena, A., "Elevated Temperature Crack Growth Rate Model for Ni-base Superalloys,"
Proceedings of the 12th International Conference on Fracture, Ottawa, Canada, July 12-17, 2009.



Effects on Crack Growth



Data Representation

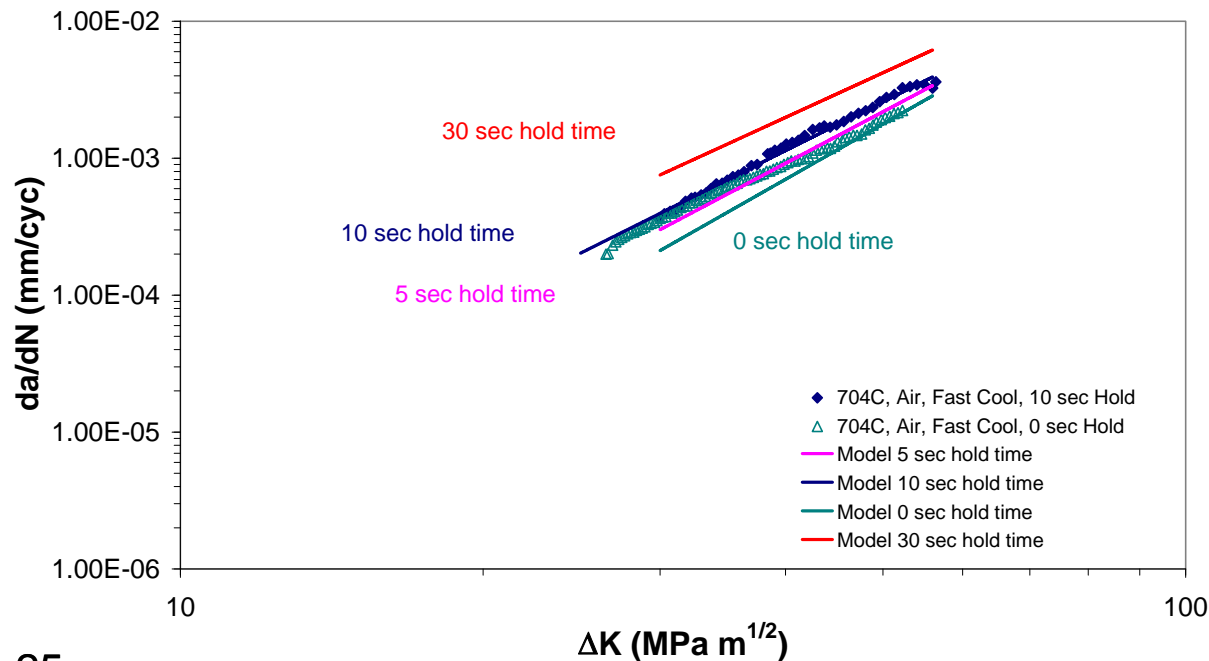
Example:

- ME3 Data, Fast Cooled, Temp = 704°C, Lab Air, 10 sec Hold Time

Assume:

- da/dt is constant with time, $(da/dN)_{td} = t_h(da/dt)_{avg}$

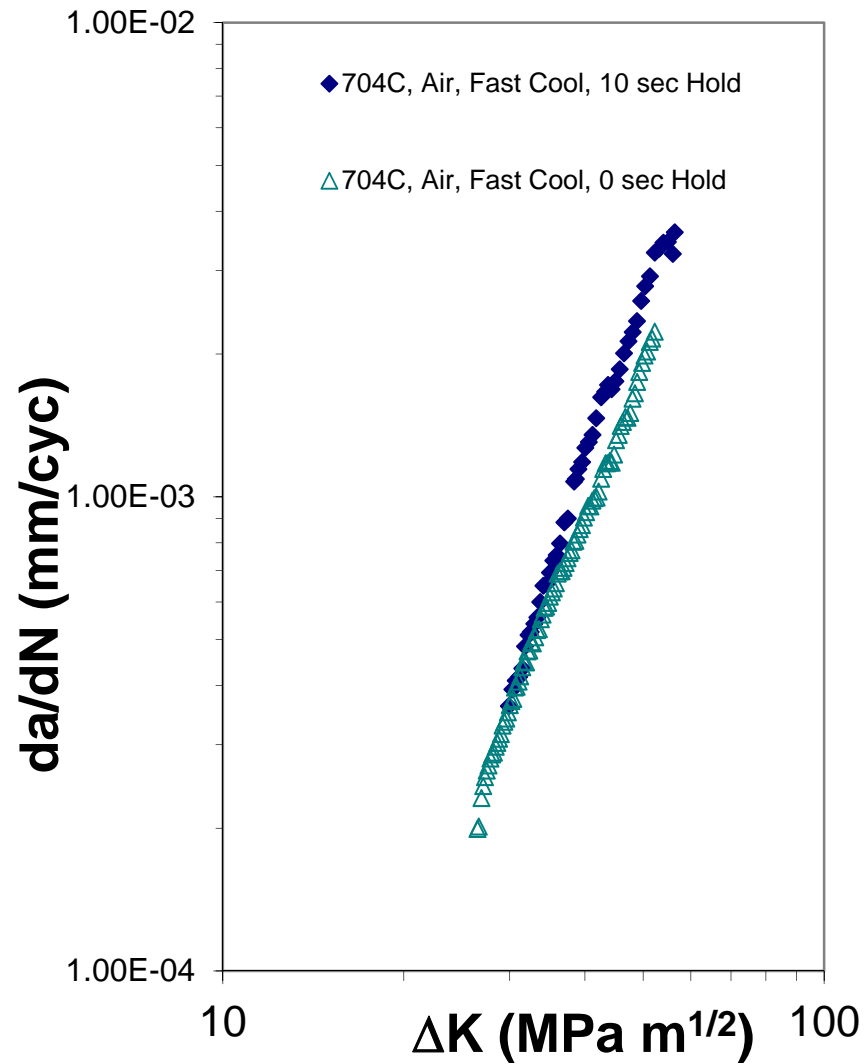
$$\left(\frac{da}{dN}\right)_{tot} = 7.51 \times 10^{-12} \Delta K^{4.62} + 1.23 \times 10^{-8} \Delta K^{4.00} \exp\left(-\frac{33,455}{R_G T}\right) + 44.37 t_h \exp\left(-\frac{265,000}{R_G T}\right) \exp\left(10,222 \left(\frac{1}{T}\right) \left(\frac{\Delta K}{1-R}\right)^{\frac{2}{n+1}}\right)$$



First approximation is
in the right direction



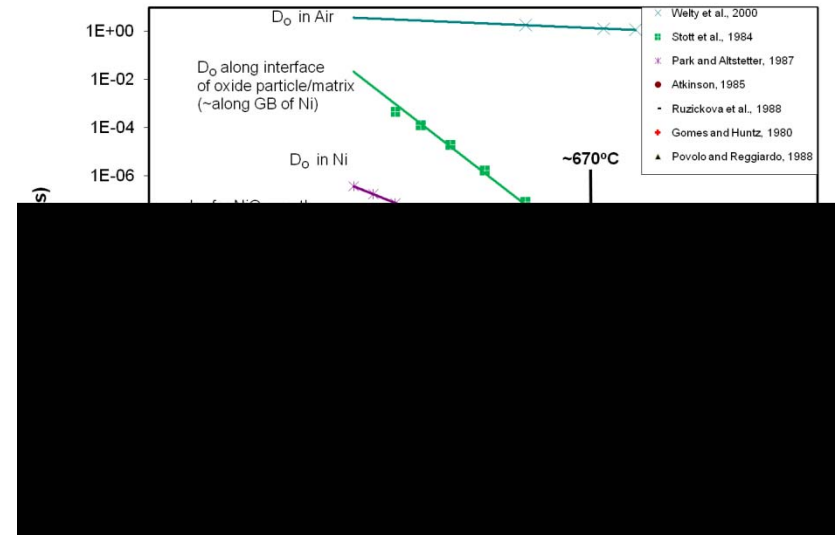
Crack Growth Data: ME3



Kinetic Chart

A. Pineau, S.D. Antolovich, *Engineering Failure Analysis* 16 (2009) 2668–2697

“...when the crack tip experiences a negative strain rate (start of unloading) the effect of oxygen is virtually eliminated. This leads to the conclusion that any heat treatment that would show more rapid relaxation at the crack tip (i.e. more rapid primary creep) would reduce the sensitivity of IN 718 to environmental attack.”



Reaction rate of TiO, grain boundary diffusion rate, and strain flux converge at ~670°C