

# New Mechanistic Models of Creep-Fatigue Interactions for Gas Turbine Components (DE-FE0011796)

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# TEAM - DOE

## Purdue University

- Thomas Siegmund with Dr. Trung Nugyen (post doc)
- Vikas Tomar with Devendra Verma (PhD student)

## Oregon State University

- Jay Kruzic with Halsey Ostergaard (PhD Student)

## DOE-NETL Program Management

- PM Dr. Rin Burks

## DOE-NETL Collaboration

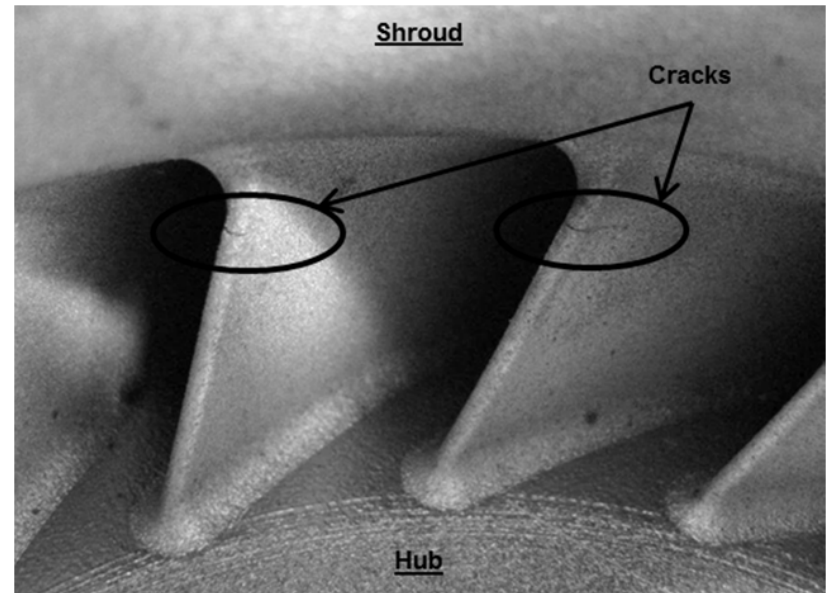
- Dr. Jeff Hawk NETL Albany

# TIMELINE

Project Milestone Description	Project Duration - Start: 2/15/2015 End: 12/1/2017												Planned Start Date	Planned End Date	Actual Start Date	Actual End Date
	Project Year (PY) 1				Project Year (PY) 2				Project Year (PY) 3							
	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12				
Project Management Plan	x												2/15/15	3/1/15	2/15/15	3/1/15
Literature Assessment	x	x											2/15/15	5/1/15	2/15/15	5/1/15
Material Acquisition	x	x											2/15/15	5/1/15	2/15/15	5/1/15
Definition of Strain Gradient Visco-Plasticity	x	x	x										2/15/15	7/1/15	2/15/15	7/1/15
Definition of Cohesive Zone Model			x	x									7/1/15	12/1/15	7/1/15	
HT Nanoindentation		x	x	x									5/1/15	12/1/15	8/1/15	
Uniaxial Cyclic Deformation Data and Parameters		x	x	x									5/1/15	12/1/15	8/1/15	
Model Implementation of UMAT and UEL				x	x	x							12/1/15	5/1/16	8/1/15	
Model Verification				x	x	x							12/1/15	5/1/16	8/1/15	

# BACKGROUND

## Cracks: In conventional and AM parts



[1] 2006 Los Angeles Incident, PROBABLE CAUSE: "The HPT stage 1 disk failed from an intergranular fatigue crack ...."

<http://aviation-safety.net/database/record.php?id=20060602-0>

[2] Direct Metal Laser Sintering: Karl Wygant et al.; Pump and Turbine 2014



# BACKGROUND

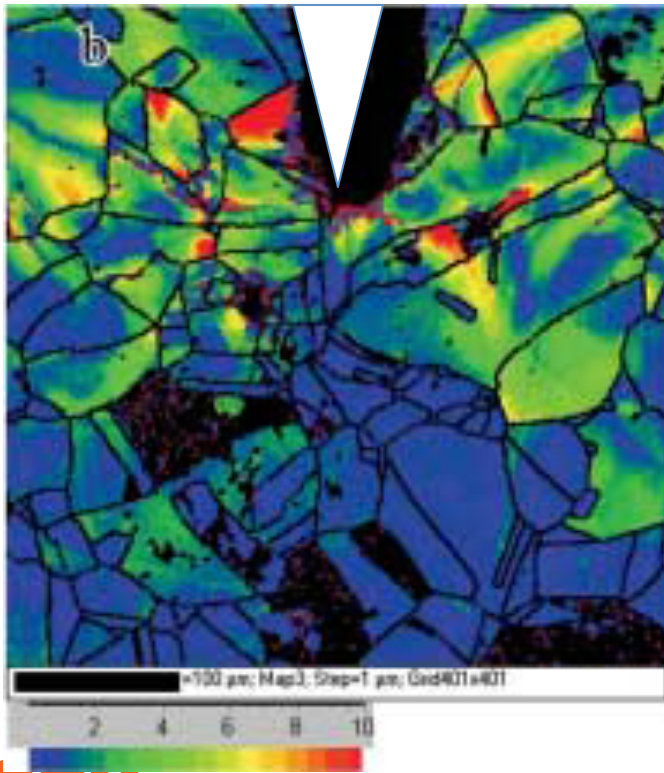
## Views on Fatigue Failure

- $S-N$ : stress only, no cracks
- Fracture Mechanics: global description, cracks  
Rule based (Paris law and beyond)
- **Micromechanics: local description**  
**Aims to avoid rules and become predictive**  
**in complex loading scenarios**

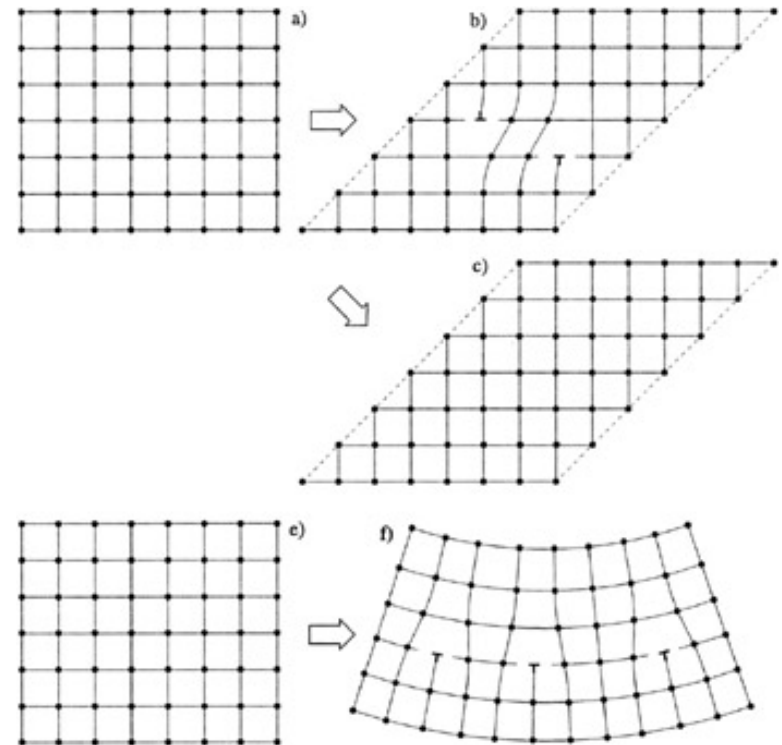
# BACKGROUND

## Plasticity

EBSD misorientation to reference at crack tip



Misorientation=GND  
Strain gradients



# BACKGROUND: RATE INDEP.

$$r_m = \frac{1}{3\pi} \frac{K}{(\sigma_0)^2} \rightarrow r_c = \frac{1}{3\pi} \frac{K}{(4\sigma_0)^2} \quad \text{.....cyclic plastic zone size}$$

$$\eta = \frac{\Delta \varepsilon_{pl}}{r_c} \quad \text{..... strain gradient, therefore a length } \Lambda [m]$$

$$\varepsilon_{pl}, \eta \rightarrow \sigma_0 = f(\varepsilon_{pl}, \eta, \text{microstr.})$$

$$\Delta a \approx \Delta CMOD = \frac{J}{2\sigma_0} \rightarrow \left( \frac{J}{2\sigma_0} / \Lambda \right) \text{.....non-dim.}$$

# BACKGROUND

## Hypothesis

**Strain Gradient effects of viscoplastic deformation play a relevant role in the failure response of IN 718 at use temperature (650°C).**

- Conventional viscoplasticity is incomplete in its description of rate dependent deformation as effects of gradients of strain are ignored.
- Gradient theories predict higher crack tip stresses, and thus stronger activation of stress dependent processes
- Gradient theories alter the tip deformation fields, and thus not only a cyclic plastic zone but also a cyclic gradient zone exist in fatigue

# BACKGROUND

## Research Question 1

**How do we formulate a constitutive framework that accounts for gradient viscoplasticity and other observed specific features of plasticity in IN 718.**

# BACKGROUND

## Research Question 2

**What are the experimental methods to determine the lengthscale parameters inherent to a gradient theory through experimentation?**



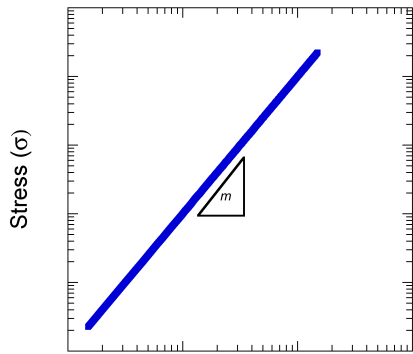
# BACKGROUND

## Research Question 3

**How is a Local-Approach to material failure best be used to predict crack growth in IN 718 under creep-fatigue-environmental loading conditions?**

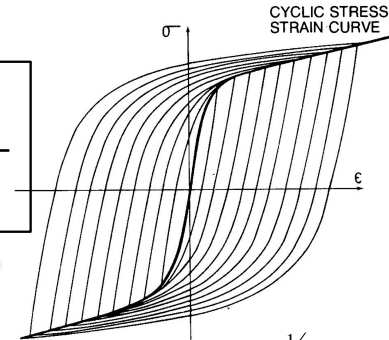
# OVERVIEW: ORIGINAL PLAN

## Research on Constitutive Parameters



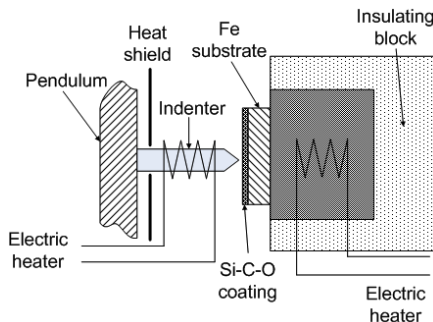
Uniaxial Creep at  
650°C  
@ multiple stress  
levels

Tensile  
cyclic stress-  
strain at  
650°C

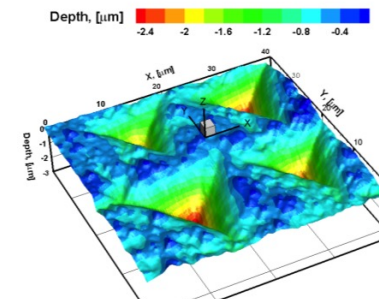


$$\frac{\Delta\epsilon}{2} = \frac{\Delta\sigma}{2E} + \left(\frac{\Delta\sigma}{2A'}\right)^{1/n}$$

Experimentally determined parameter	Symbol	Experiment
Reference stress	$A'$	Cyclic tensile tests
Cyclic strain hardening exponent	$n$	Cyclic tensile tests
Strain rate exponent	$m$	Uniaxial creep & Nanoindentation
Reference strain rate	$\dot{\epsilon}_0$	Uniaxial creep & Nanoindentation
Characteristic length scale	$l$	Nanoindentation
Dislocation-strain softening	$\rho_i$	Nanoindentation post creep

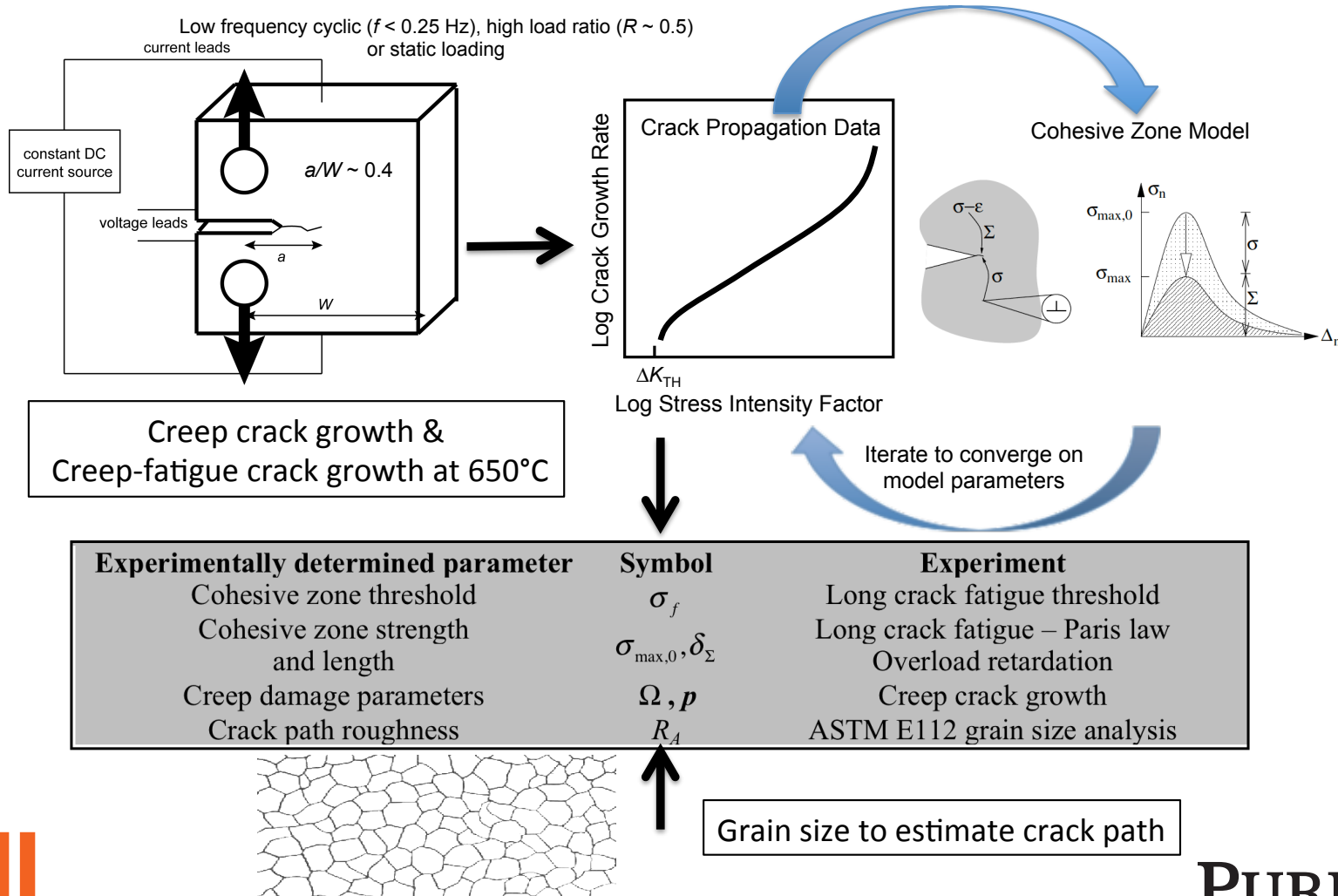


Nano-  
indentation  
at 650°C



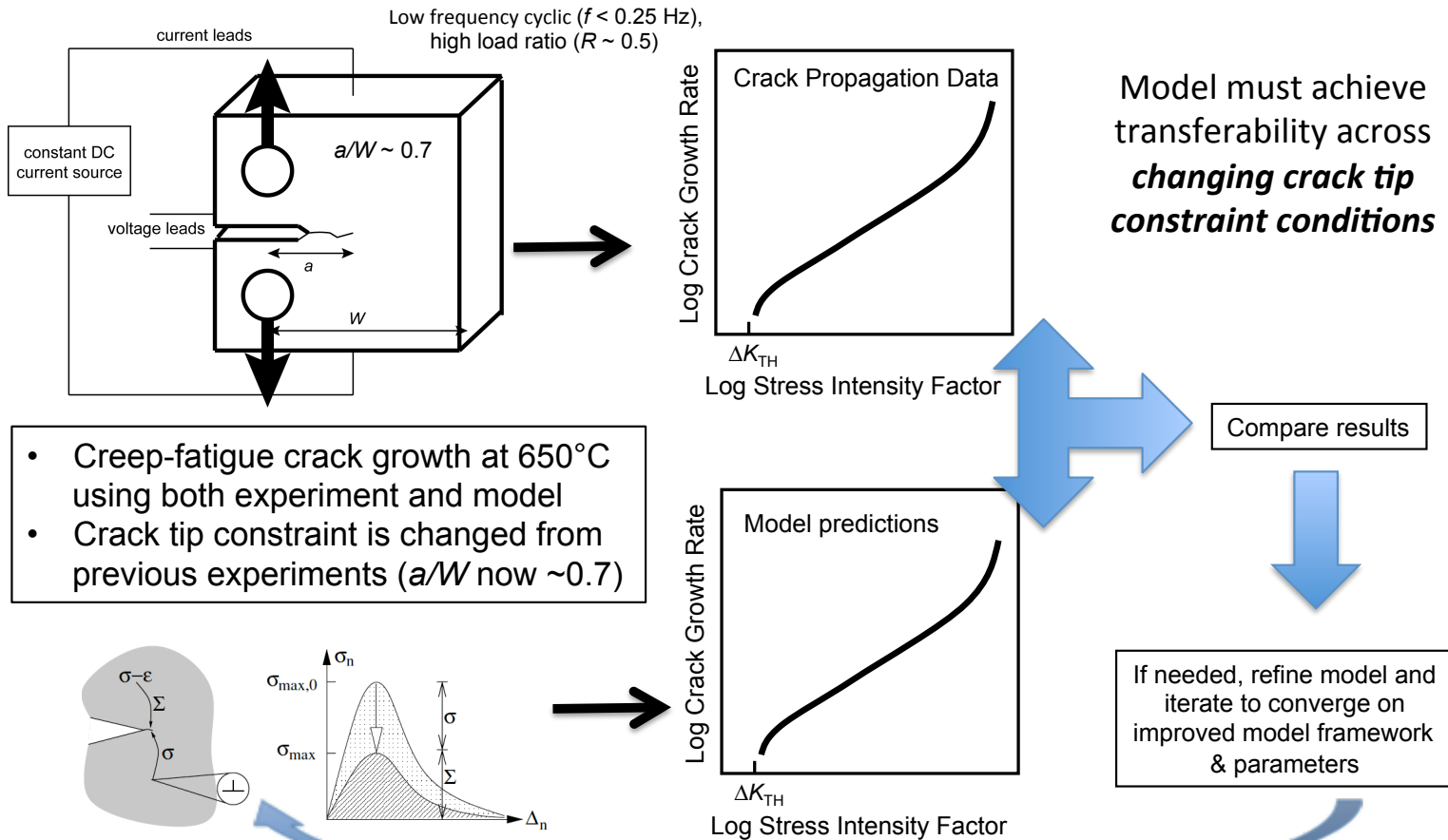
# OVERVIEW: ORIGINAL PLAN

## Research on Crack Propagation Models



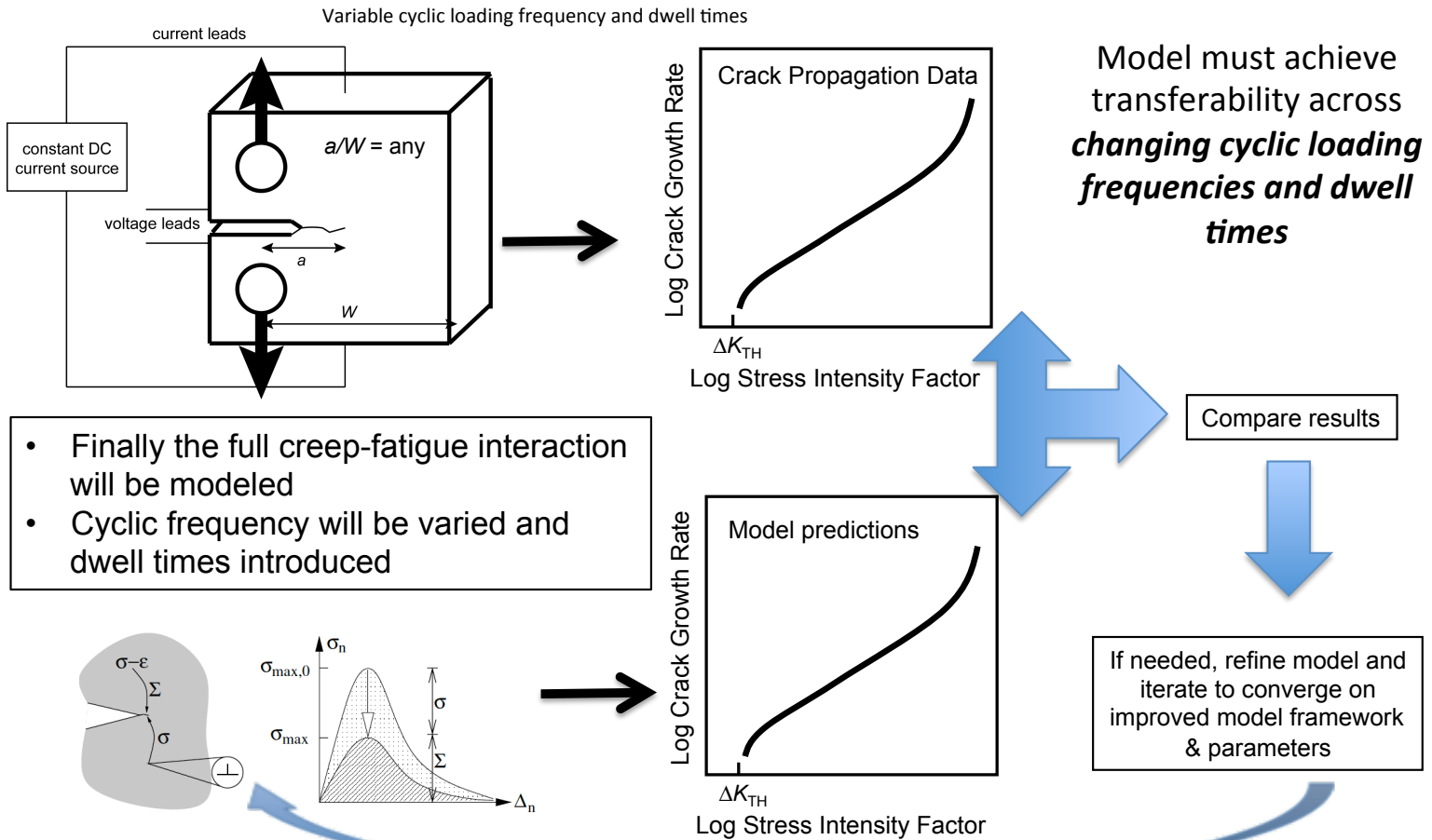
# OVERVIEW: ORIGINAL PLAN

## Initial Validation & Model Refinement



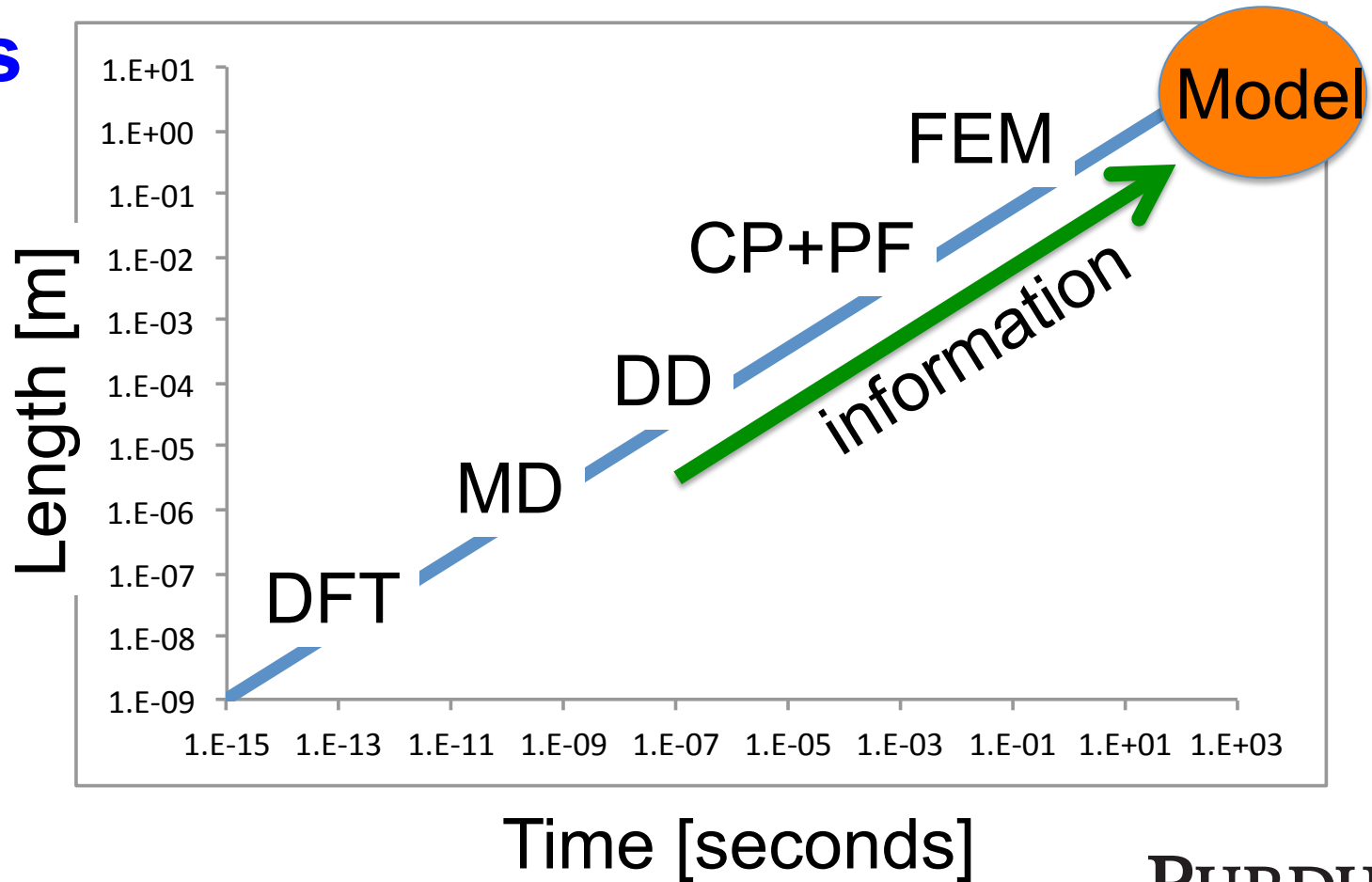
# OVERVIEW: ORIGINAL PLAN

## Final Validation & Model Refinement



# OVERVIEW: LENGTH AND TIME

**Small Scales and Long Times can only be addressed with advanced continuum models**





# PROGRESS: LEAD KRUZIC

## Material Acquisition and Collaboration

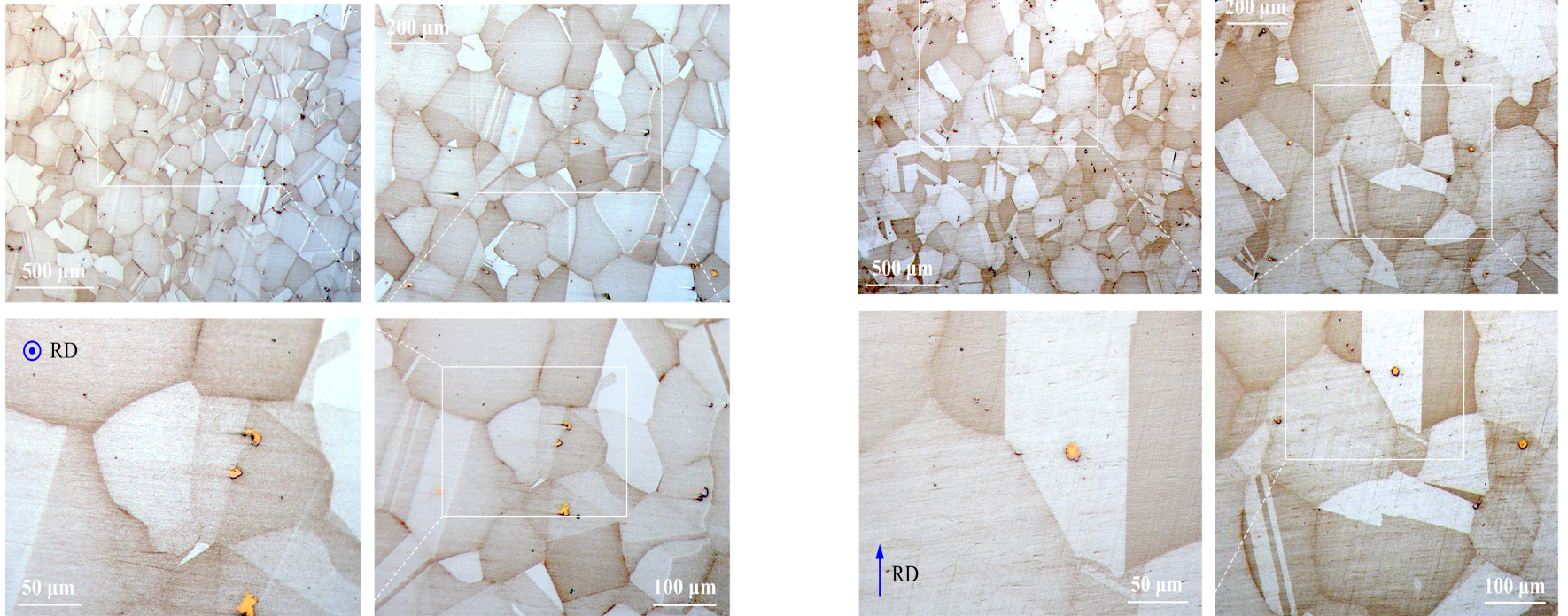
- **IN 718**
- **Provided by Jeff Hawk, NETL Albany**
- **Processing (at NETL)**

Step forging and squaring (from round slab  $D=8.5''$  to plate  $t=1.25''$ ; Hot rolling into a plate  $t=0.616''$ ; solution annealed. Received a plate roughly  $27'' \times 5 \frac{5}{8}'' \times 0.616''$ .
- **Processing (at OSU)**

Solution annealed at  $982^{\circ}\text{C}$ , 1hr, air cooled Hardened by holding at  $718^{\circ}\text{C}$  for 8hrs, then furnace cooled to  $621^{\circ}\text{C}$  and held for 10 hrs, then air cooled.

# PROGRESS

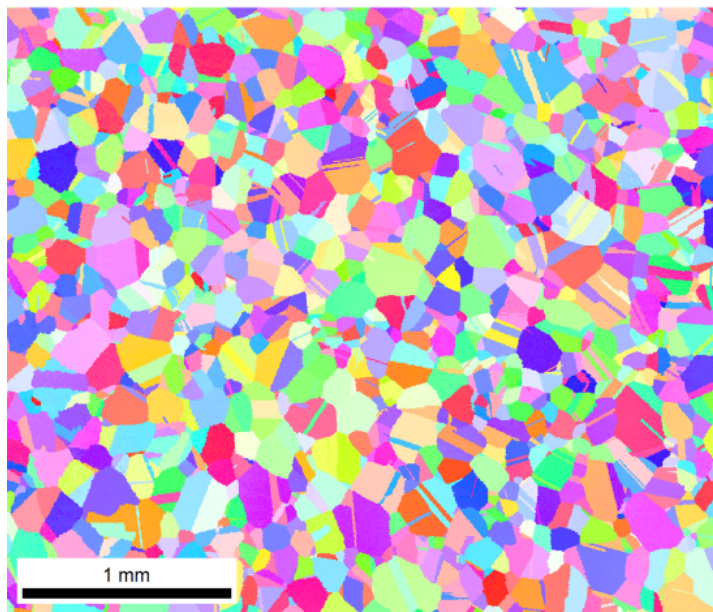
## Optical Microstructure Characterization



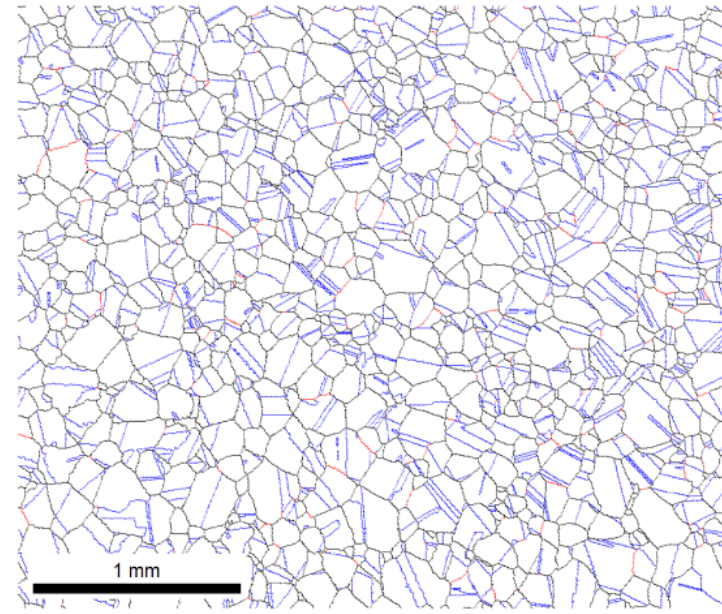
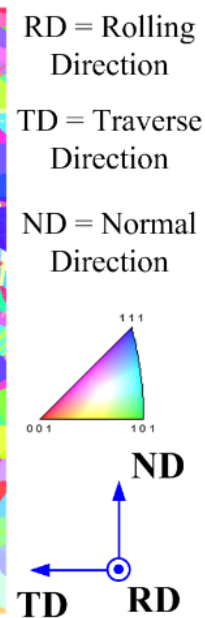
**Uniform and equiaxed microstructure**

# PROGRESS

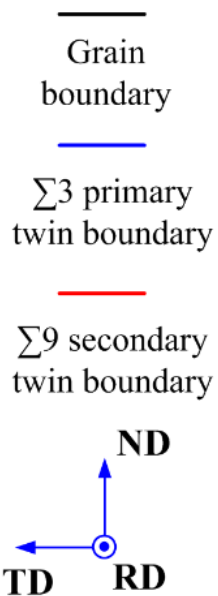
## EBSD on Transverse Section



(a) Crystal orientation map



(b) Grain/twin boundary map



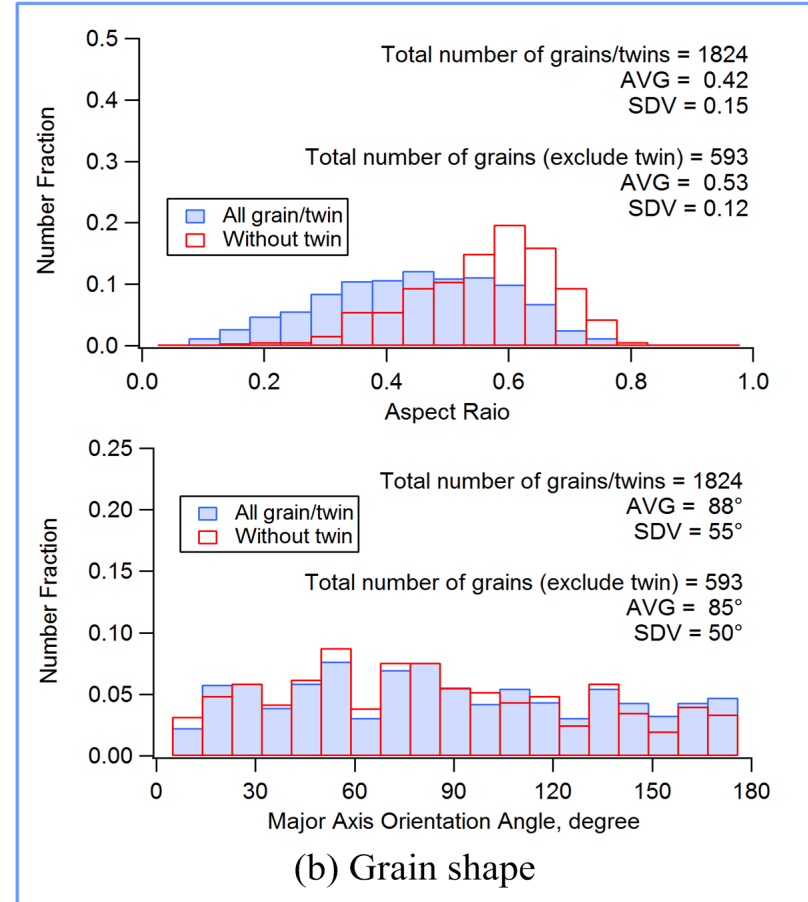
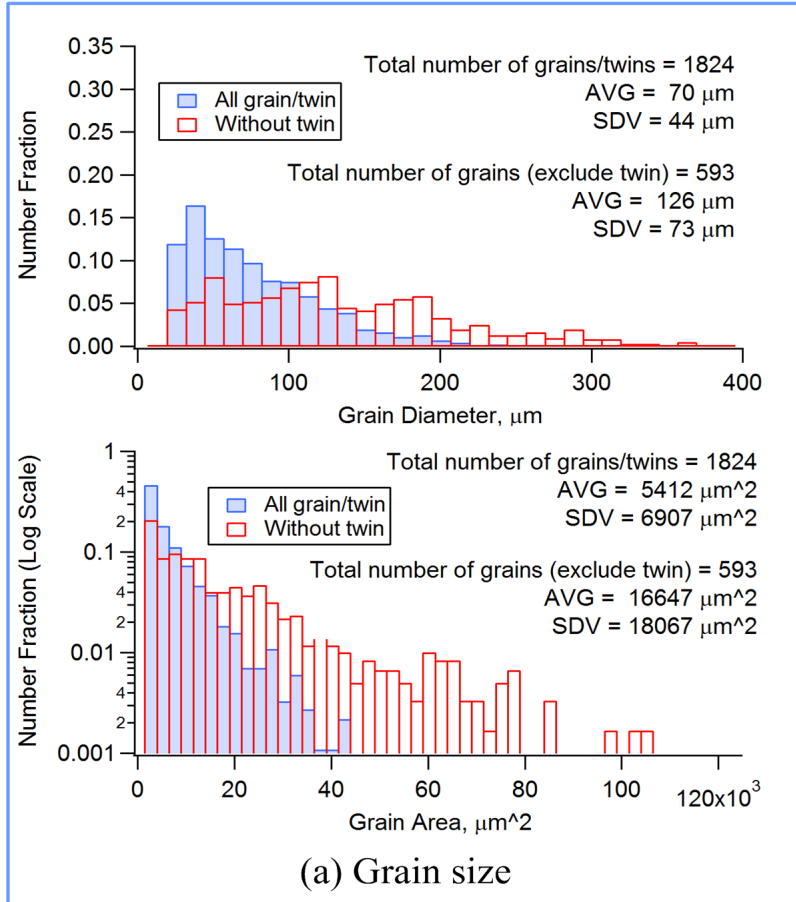
**Highly twinned**

**Most twins as  $\Sigma 3$  (from recrystallization)**



# PROGRESS

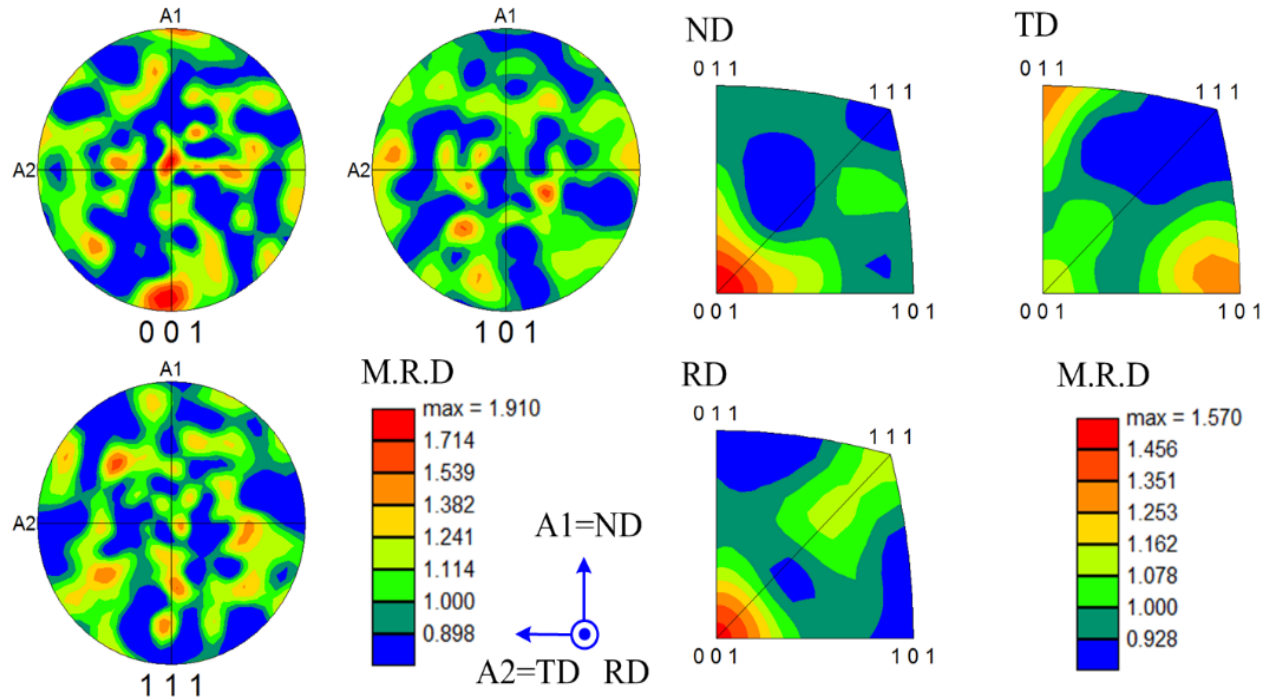
## Grains & Twins: Grain Size and Orientation



Analysis with and without twins

# PROGRESS

## Texture



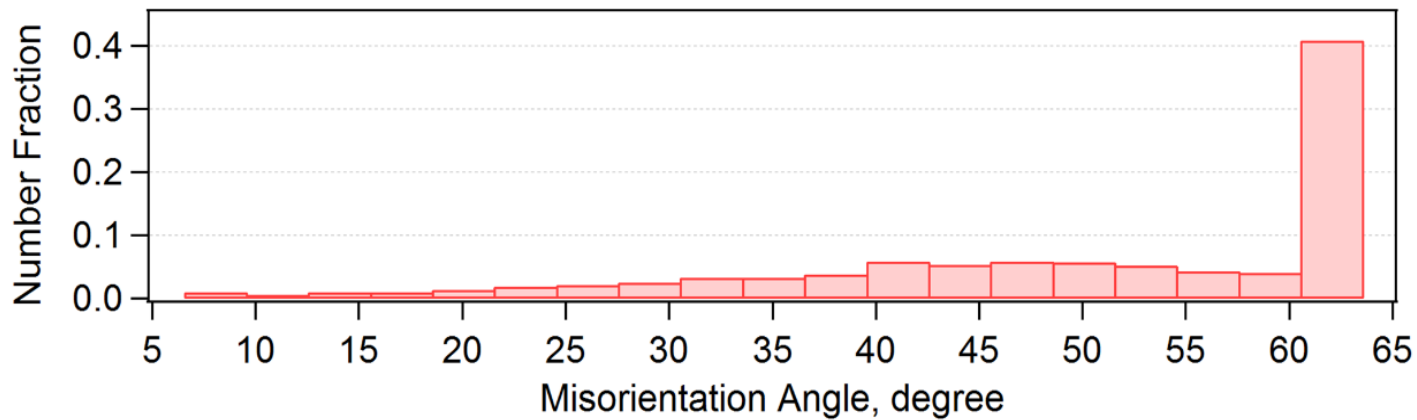
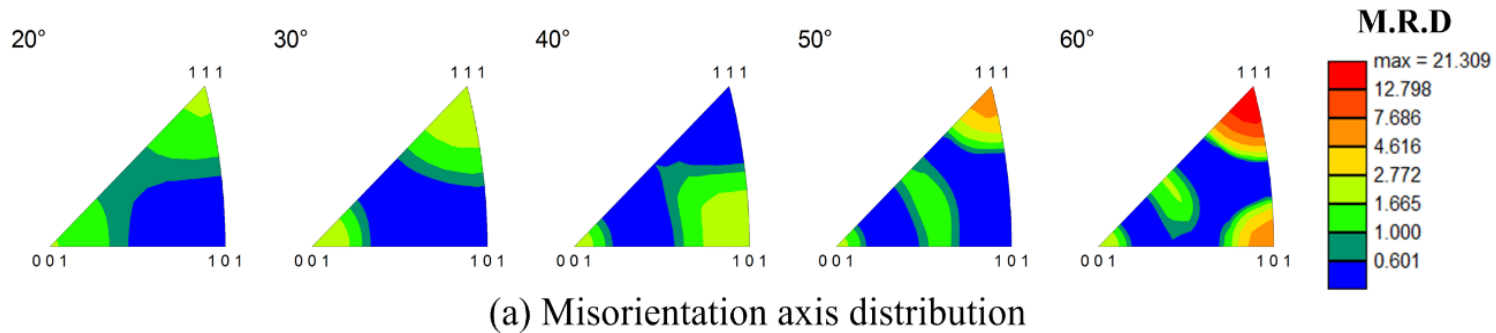
(a) Pole figure

(b) Inverse pole figure

**Only weak initial texture, remnants of a cube (100)[001] and even weaker fiber  $\langle 111 \rangle$  texture exist**

# PROGRESS

## Grain and Twin Boundaries

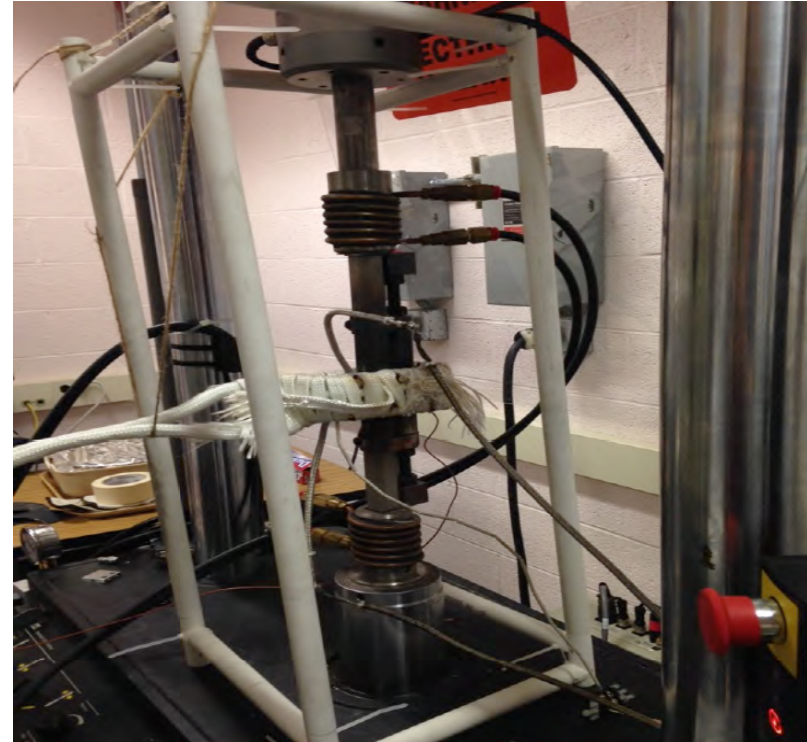
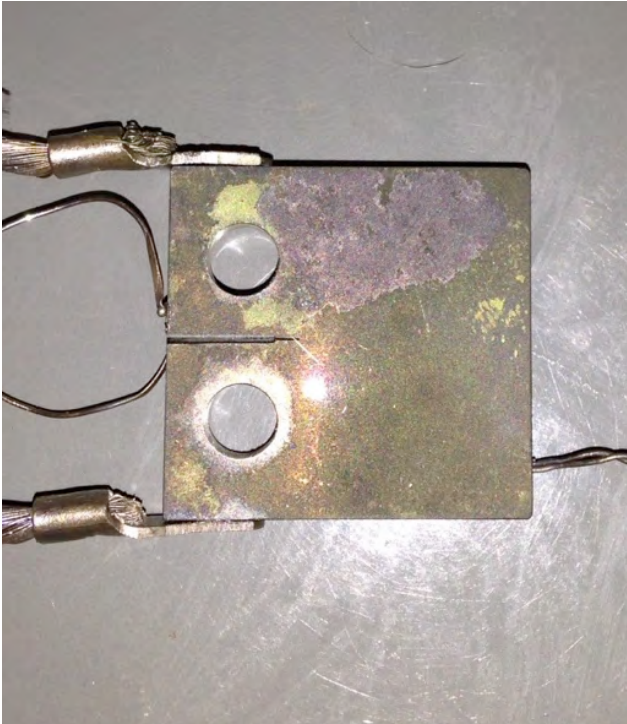


**Strongly influenced by S3 twins**



# PROGRESS

## Creep Experiment: In progress

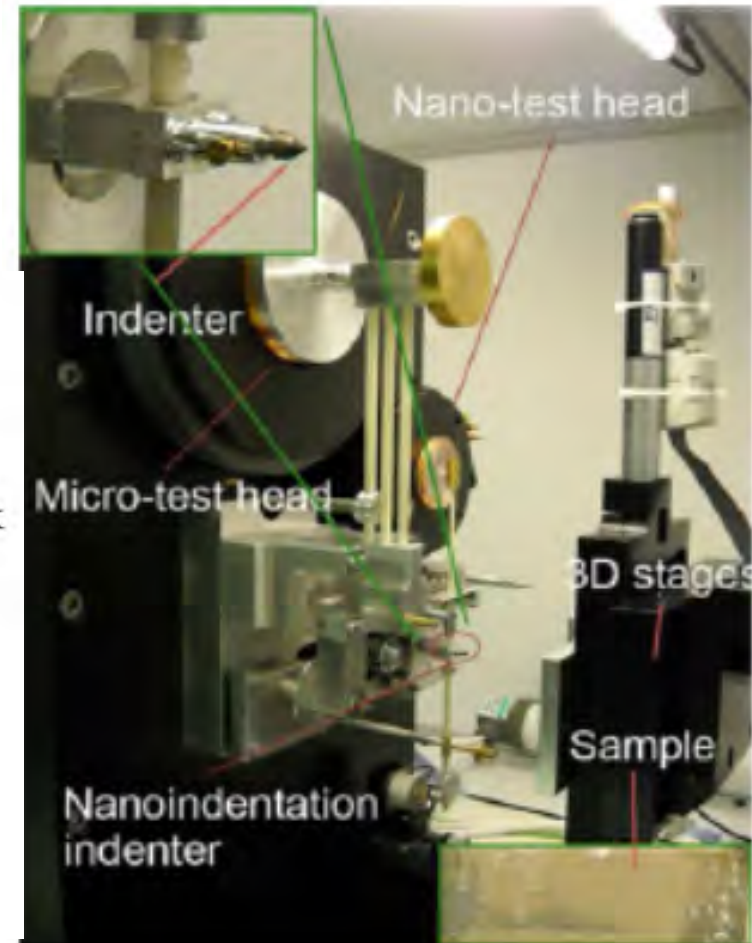
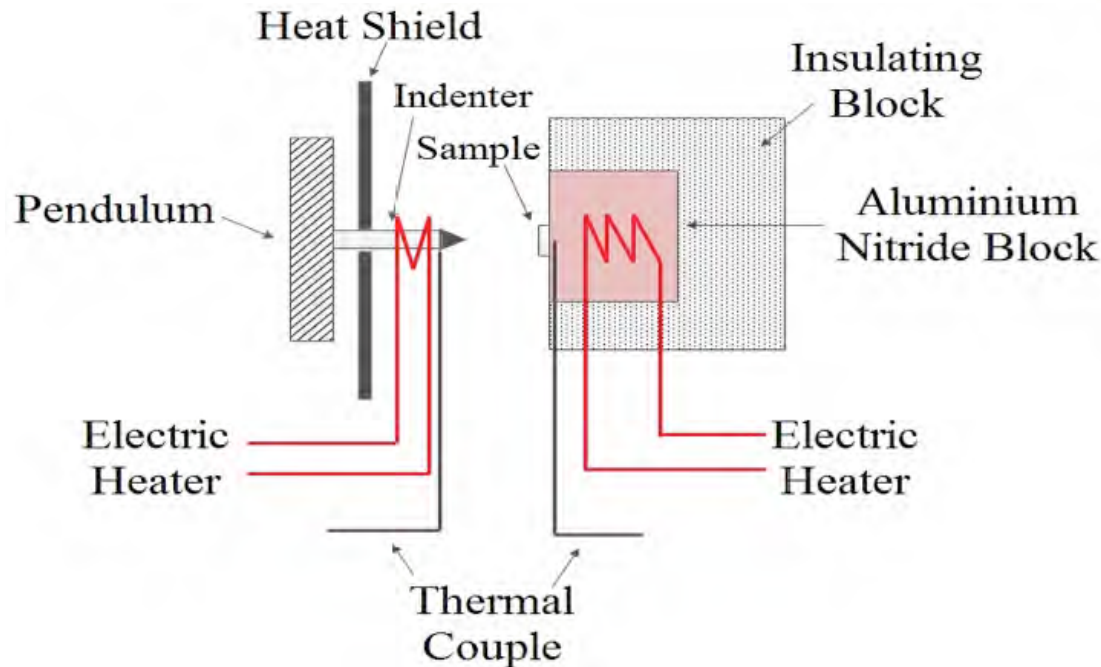


HT Experiments on CT specimens with potential drop measurements

# PROGRESS: LEAD TOMAR

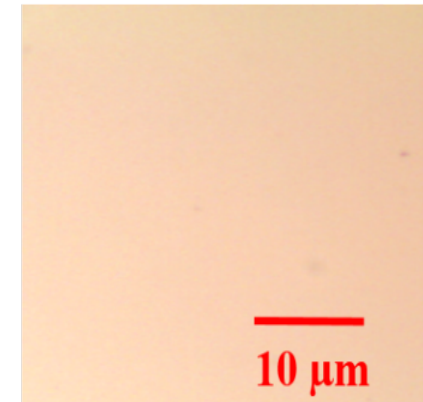
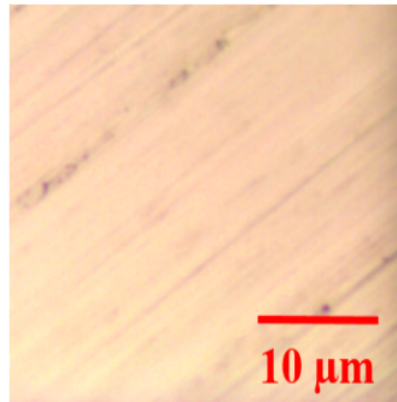
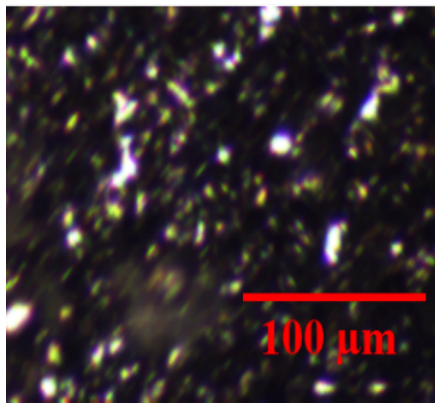
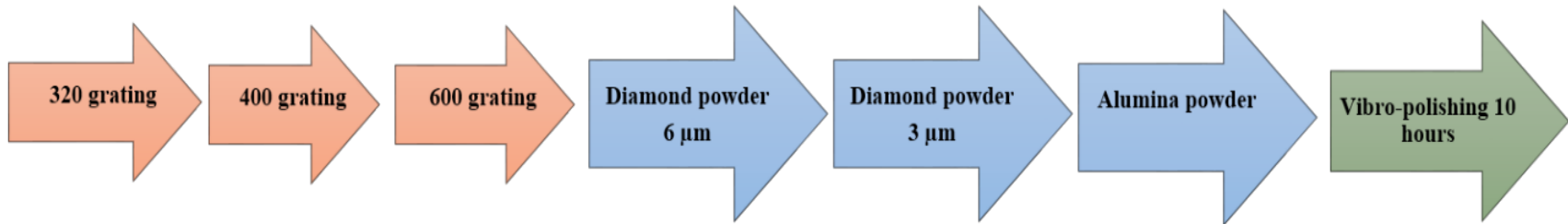
## High Temperature Nanoindentation

Probe plasticity at small length scales



# PROGRESS

## HT Nanoindentation: Specimen preparation



# PROGRESS

## HT Nanoindentation: Experimental plan

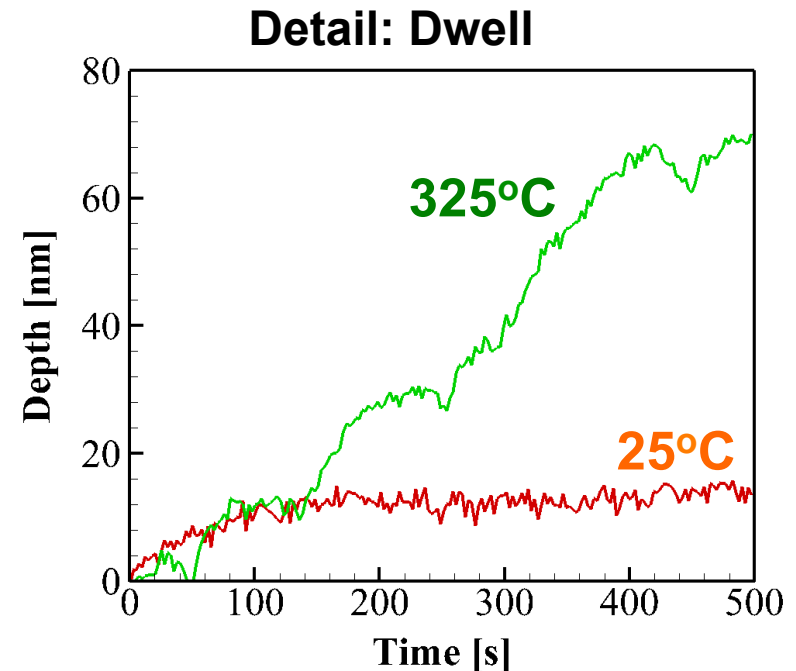
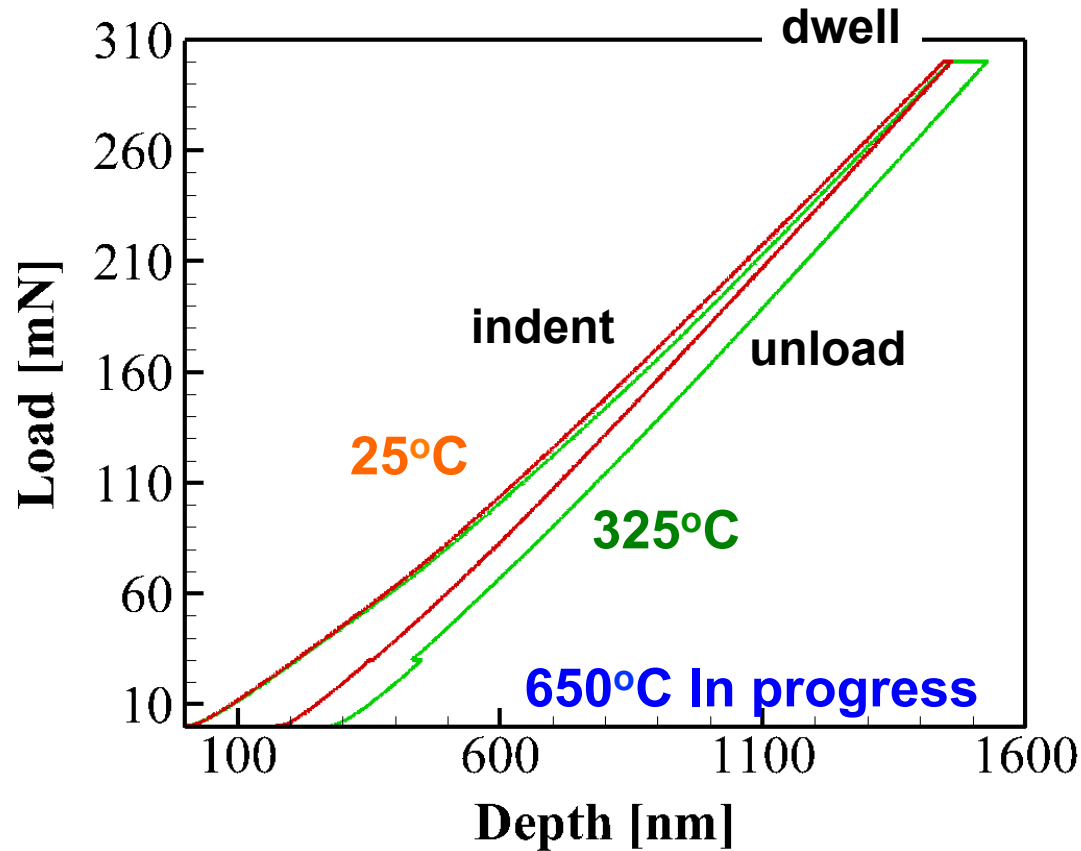
Through change in indent depth the ratio of **viscoplast. strain & viscoplast. strain gradient** is altered → obtain the relevant length scale

Load (mN)	25 °C (no. of points)	350 °C (no. of points)	650 °C (no. of points)	Post oxidation (no. of points)	Dwell time (s)
50	10	10	10	10	500
100	10	10	10	10	500
200	10	10	10	10	500
300	10	10	10	10	500
400	10	10	10	10	500



# PROGRESS

## HT Nanoindentation: 1<sup>st</sup> data on IN 718



# PROGRESS: LEAD SIEGMUND

## Constitutive Models: Gradient Effects

### Flow stress

$$\sigma_{\text{flow}} = \sigma_0 + M\alpha\mu b\sqrt{\rho}$$

$\sigma_0$ : stress related to lattice friction and solute contents

$M$ : average Taylor factor ( $M \approx 3$ )

$\alpha$ : weighting factor of dislocation interactions ( $\alpha \approx 1/3$ )

$\mu$ : shear modulus

$b$ : Burgers vector



# PROGRESS

## Constitutive Models

Dislocation density:  $\rho = \rho_S + \rho_G$

- Statistically stored dislocation:

$$\rho_S = \frac{\sqrt{3}\bar{\epsilon}^{vp}}{b\Lambda}$$

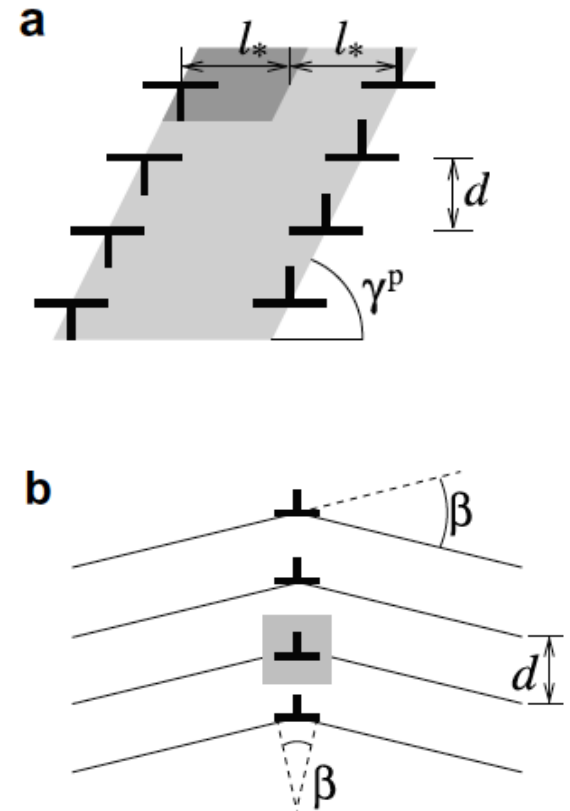
$\Lambda$ : mean free path

- Geometrically necessary dislocation:

$$\rho_G = \bar{r} \frac{\bar{\eta}}{b}$$

$\bar{\eta}$ : effective plastic strain gradient

$\bar{r}$ : Nye-factor ( $\bar{r} = 1.90$ )



# PROGRESS

## Constitutive Models: Flow Stress

$$\sigma_{\text{flow}} = \sigma_0 + M \alpha \mu b \sqrt{\rho_S + \rho_G} = \sigma_0 \left( 1 + \frac{\sqrt{3} \alpha \mu b}{\sigma_0} \sqrt{\frac{\sqrt{3} \bar{\epsilon}^{vp}}{b \Lambda} + \frac{\bar{\eta}}{b}} \right)$$

$$\Delta \dot{\bar{\epsilon}}^{vp} = g(\boldsymbol{\sigma}, \mathbf{q}) \quad \mathbf{q}: \text{state variable vector}$$

$$\Delta \bar{\epsilon}^{vp} = \Delta t \dot{\bar{\epsilon}}^{vp} = \Delta t \cdot g(\boldsymbol{\sigma}, \mathbf{q}) = \Delta t \dot{\bar{\epsilon}}_0 \left( \frac{\bar{\sigma}}{\sigma_{\text{flow}}} \right)^m$$

$$\left( \frac{J}{2\sigma_0} / \Lambda \right), (b / \Lambda), \left( \frac{j}{2\sigma_y} / \dot{\bar{\epsilon}}_0 \Lambda \right)$$

# PROGRESS

## Computational Implementation

$$\dot{\epsilon}_{ij} = \frac{\dot{\sigma}_{ij}}{9K} \delta_{ij} + \frac{\dot{s}_{ij}}{2\mu} + \frac{3\dot{\bar{\epsilon}}^{vp}}{2\bar{\sigma}} \dot{s}_{ij} = \frac{\dot{\sigma}_{ij}}{9K} \delta_{ij} + \frac{\dot{s}_{ij}}{2\mu} + \frac{3\dot{\bar{\epsilon}}_0}{2\bar{\sigma}} \left( \frac{\bar{\sigma}}{\sigma_0 \left( 1 + \frac{\sqrt{3}\alpha\mu b}{\sigma_0} \sqrt{\frac{\sqrt{3}\bar{\epsilon}^{vp}}{b\Lambda} + \frac{\bar{\eta}}{b}} \right)} \right)^m \dot{s}_{ij}$$

$$\dot{\sigma}_{ij} = K\dot{\epsilon}_{ij}\delta_{ij} + 2\mu \left\{ \dot{\epsilon}'_{ij} - \frac{3\dot{\bar{\epsilon}}_0}{2\bar{\sigma}} \left[ \frac{\bar{\sigma}}{\sigma_0 \left( 1 + \frac{\sqrt{3}\alpha\mu b}{\sigma_0} \sqrt{\frac{\sqrt{3}\bar{\epsilon}^{vp}}{b\Lambda} + \frac{\bar{\eta}}{b}} \right)} \right]^m \dot{s}_{ij} \right\}$$

# PROGRESS

## Computational Implementation

**Euler implicit scheme + Newton-Raphson iteration**

- Nonlinear equations

$$f_1(\Delta\bar{\boldsymbol{\varepsilon}}^{vp}, \bar{\boldsymbol{\sigma}}) = \Delta\bar{\boldsymbol{\varepsilon}}^{vp} - \Delta t \dot{\bar{\boldsymbol{\varepsilon}}}_0 \left( \frac{\bar{\boldsymbol{\sigma}}}{\sigma_{\text{flow}}} \right)^m = 0$$

$$f_2(\Delta\bar{\boldsymbol{\varepsilon}}^{vp}, \bar{\boldsymbol{\sigma}}) = 3\mu(\bar{\boldsymbol{\varepsilon}}^* - \Delta\bar{\boldsymbol{\varepsilon}}^{vp}) - \bar{\boldsymbol{\sigma}} = 0$$

- Trial state

$$\boldsymbol{\varepsilon}_{n+1}^{trial} = \boldsymbol{\varepsilon}_n^{el} + \Delta\boldsymbol{\varepsilon}; \quad \bar{\boldsymbol{\varepsilon}}^* = \sqrt{\frac{2}{3} \boldsymbol{\varepsilon}_{n+1}^{trial} : \boldsymbol{\varepsilon}_{n+1}^{trial}}$$

# PROGRESS

## Computational Implementation

- Iteration

$$\begin{Bmatrix} \Delta \bar{\epsilon}^{vp} \\ \bar{\sigma} \end{Bmatrix}_{n+1} = \begin{Bmatrix} \Delta \bar{\epsilon}^{vp} \\ \bar{\sigma} \end{Bmatrix}_n - \mathbf{J}_n^{-1} \begin{Bmatrix} f_1(\Delta \bar{\epsilon}^{vp}, \bar{\sigma}) \\ f_2(\Delta \bar{\epsilon}^{vp}, \bar{\sigma}) \end{Bmatrix}_n$$

$$\mathbf{J}_n = \begin{bmatrix} \frac{\partial f_1}{\partial \Delta \bar{\epsilon}^{vp}} & \frac{\partial f_1}{\partial \bar{\sigma}} \\ \frac{\partial f_2}{\partial \Delta \bar{\epsilon}^{vp}} & \frac{\partial f_2}{\partial \bar{\sigma}} \end{bmatrix}_n$$

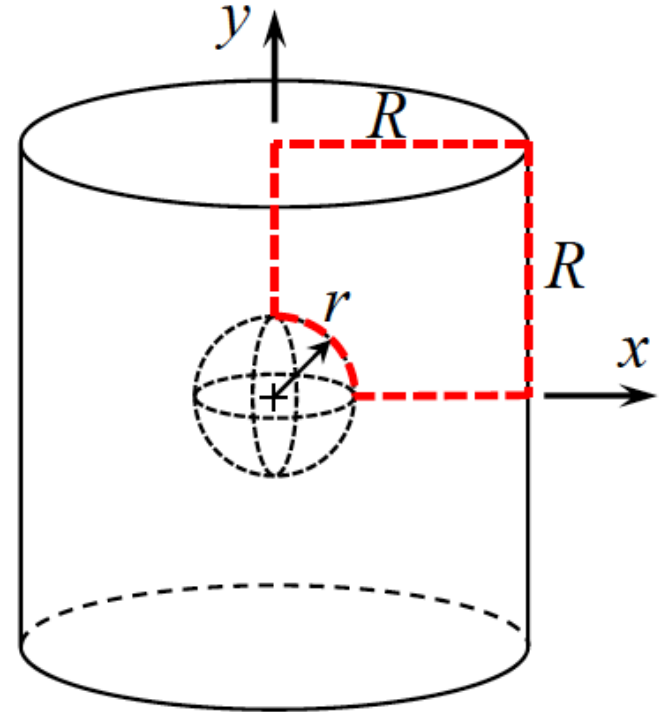
$$\bar{\epsilon}_{n+1}^{vp} = \bar{\epsilon}_n^{vp} + \Delta \bar{\epsilon}^{vp}$$

- Stress update follows a standard procedure upon convergence of the above iteration.

# OUTCOMES

## Results: Creep Rupture

Relates to issue of voids in DMLS materials

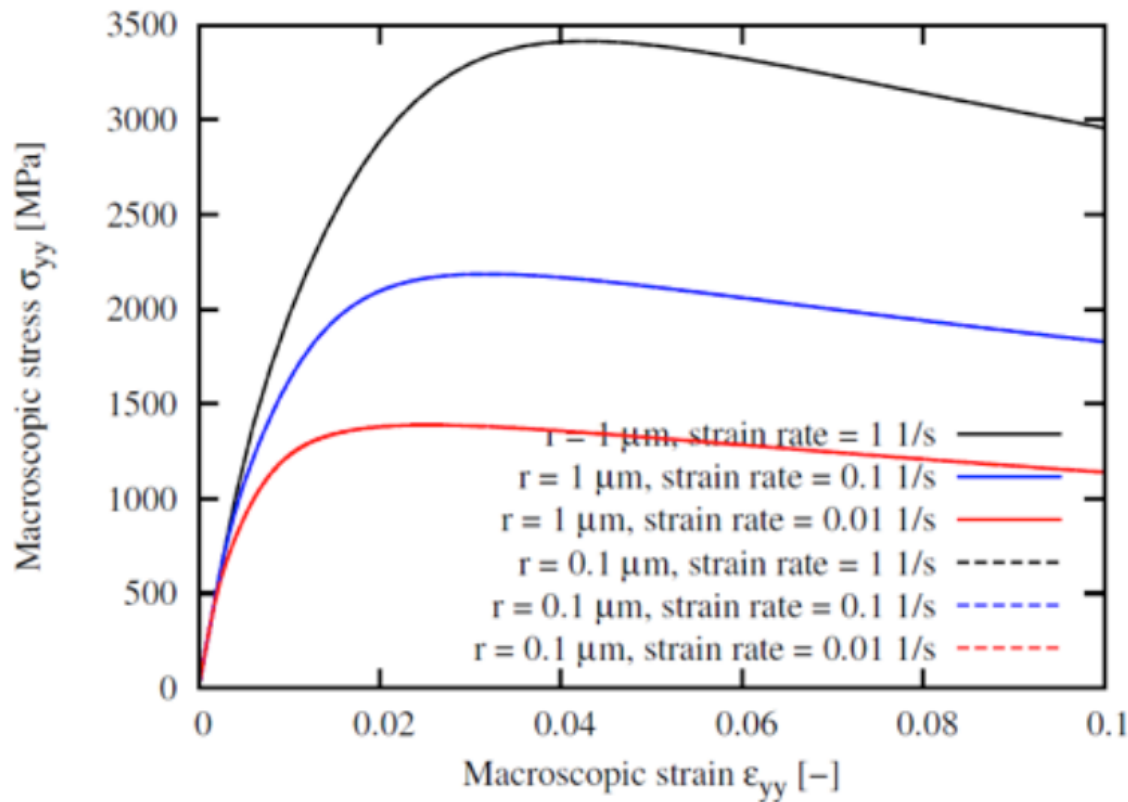


$E$ (GPa)	$\nu$	$\sigma_{y0}$ (MPa)	$\dot{\epsilon}_0$ ( $s^{-1}$ )	$m$	$b$ (nm)
200	0.3	250	0.005	5	0.25



# PROGRESS

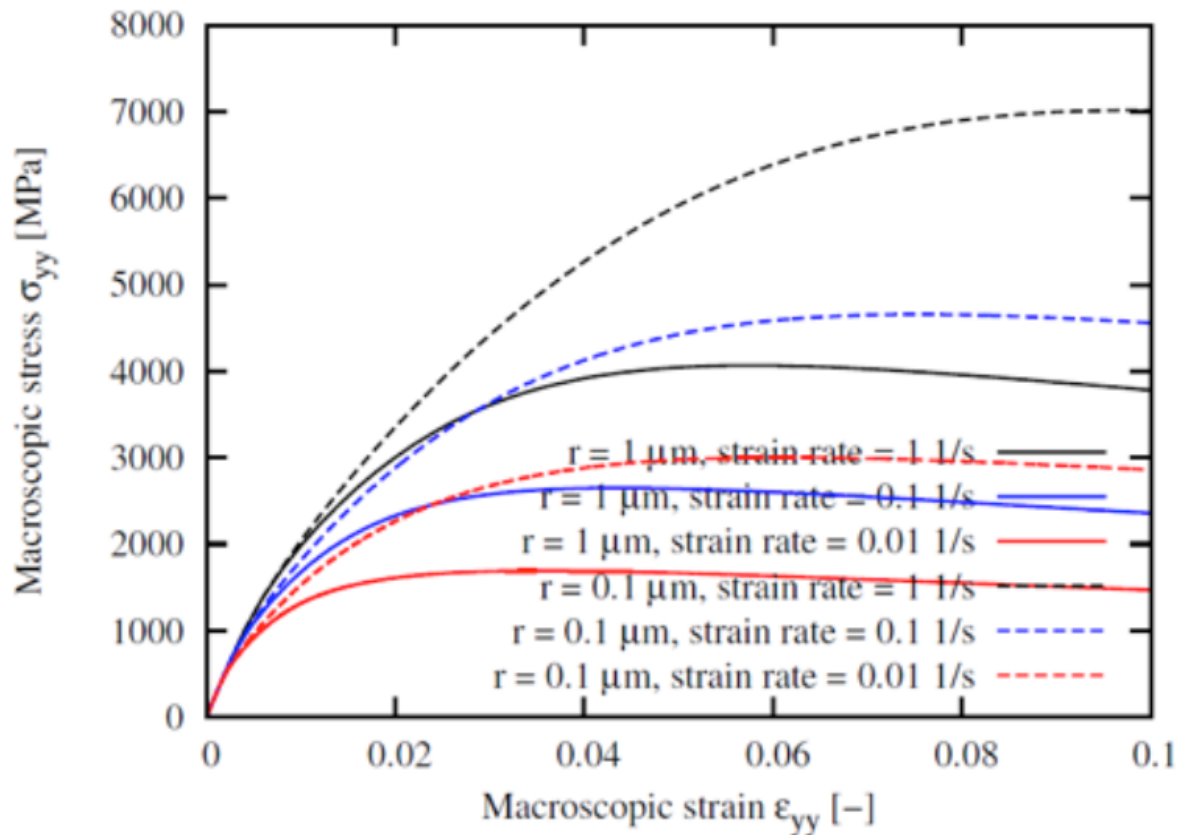
## Void Growth conventional plasticity No size effect only rate effect



# PROGRESS

## Void Growth with SGP:

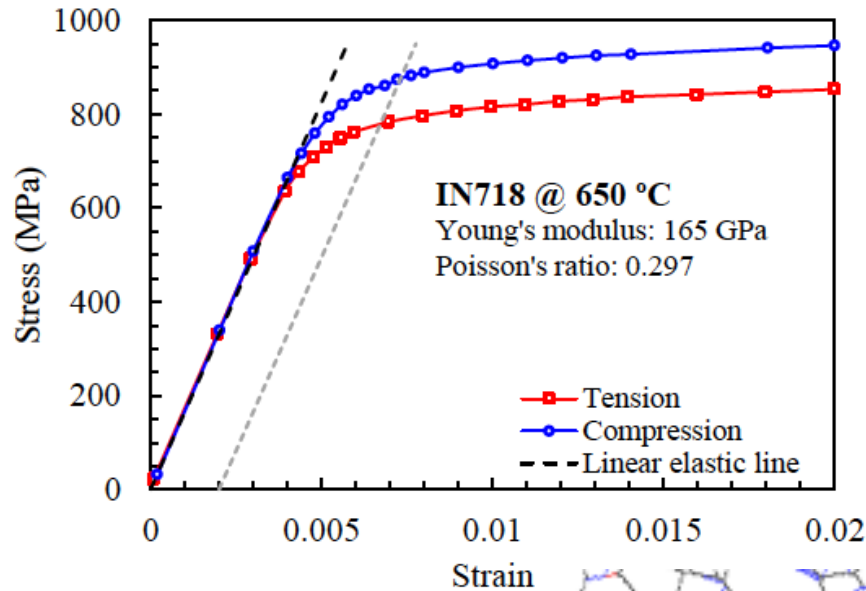
## Void Size Effect combined with a rate effect



- Smaller voids lead to higher stresses
- Smaller voids are more sensitive to rate

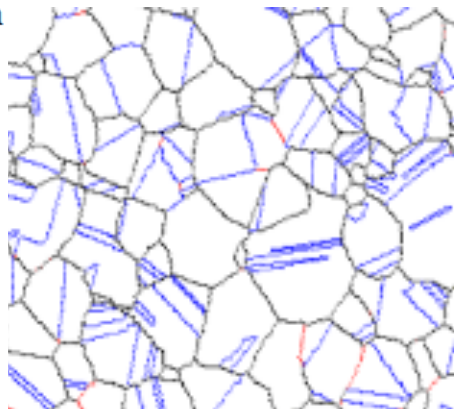
# PROGRESS

## Strength Differential Effect (Data by Lissenden et al)



$$SD = 2 \frac{|\sigma_C| - |\sigma_T|}{|\sigma_C| + |\sigma_T|} = 0.12$$

$$SR = \frac{|\sigma_T|}{|\sigma_C|} = 0.88$$



# PROGRESS

## Strength Differential Effect: Yield Function

$$\Phi(s_1, s_2, s_3) = \left( |s_1| - k \cdot s_1 \right)^m + \left( |s_2| - k \cdot s_2 \right)^m + \left( |s_3| - k \cdot s_3 \right)^m$$

$m, k$

$m = 2, k = 0 \dots$  von Mises

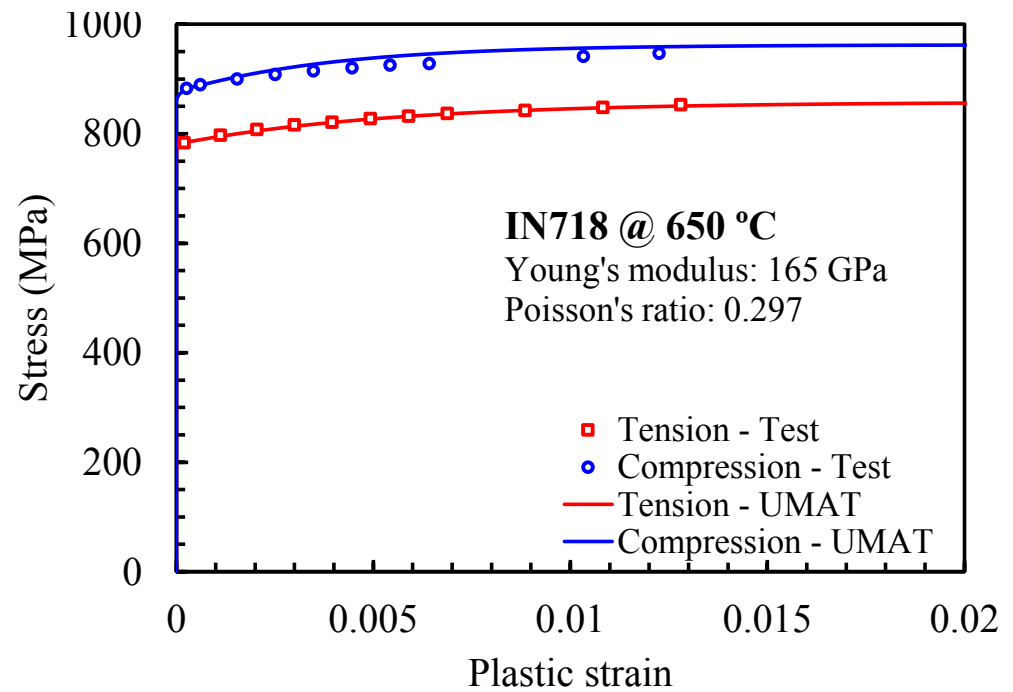
$$k = \frac{1 - \left\{ \frac{2^m - 2 \cdot (\sigma_T / \sigma_C)^m}{(2 \cdot \sigma_T / \sigma_C)^m - 2} \right\}^{(1/m)}}{1 + \left\{ \frac{2^m - 2 \cdot (\sigma_T / \sigma_C)^m}{(2 \cdot \sigma_T / \sigma_C)^m - 2} \right\}^{(1/m)}}$$

# PROGRESS

## Strength Differential Effect: UMAT

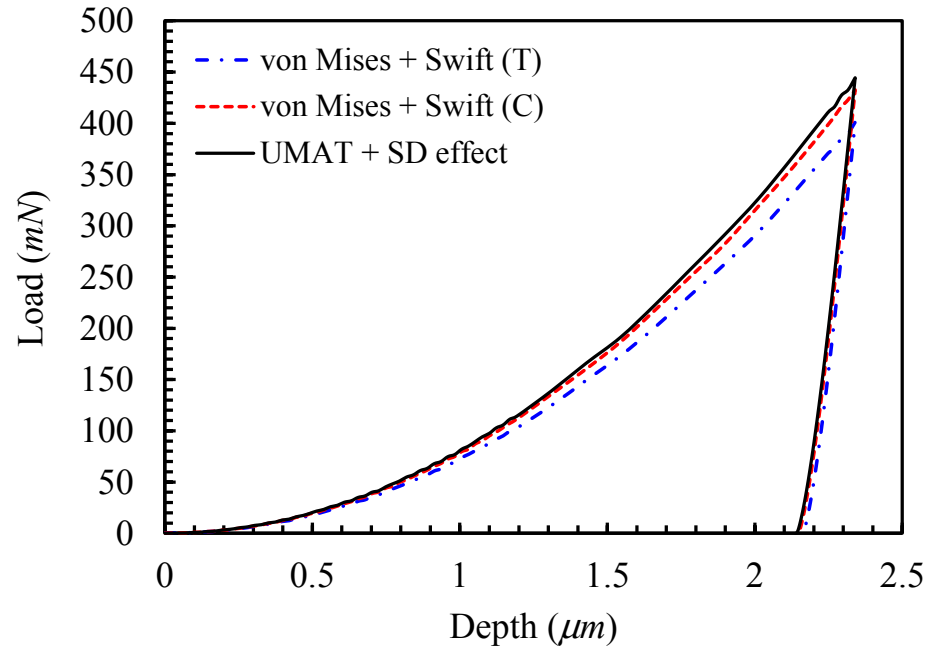
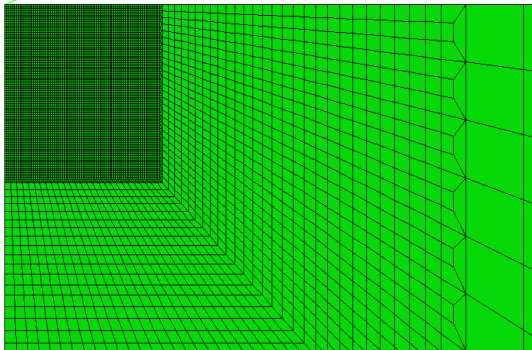
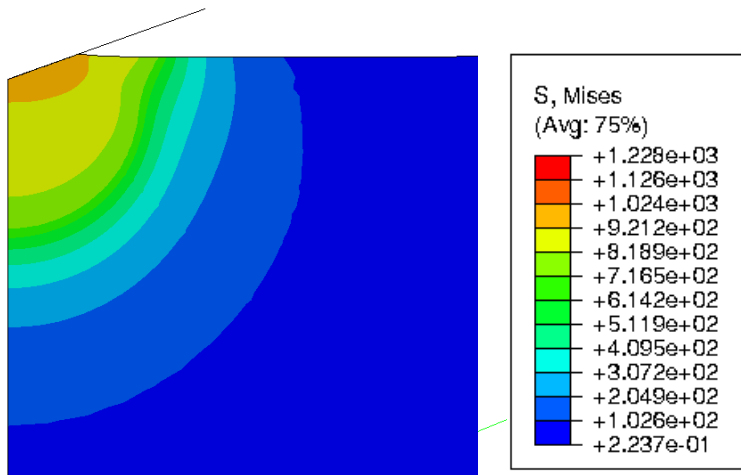
E (GPa)	$\nu$	$\sigma_T$ (MPa)	$\sigma_C$ (MPa)	K (MPa)	$\epsilon_0$	n
165	0.297	779	876	1003	0.0013	0.038

$$\sigma = K \left( \epsilon_0 + \bar{\epsilon} \right)^n$$



# PROGRESS

## Strength Differential & Indentation



Von Mises + Swift (T)	Von Mises + Swift (C)	UMAT w/ SD
1.0	1.09	1.12



# PROGRESS

## Crack Growth: Cohesive Zone Models

$$T_n = \sigma_{\max,0} e^{\left(\frac{\Delta_n}{\delta_0}\right)} \exp\left(-\frac{\Delta_n}{\delta_0}\right)$$

$$\sigma_{\max} = \sigma_{\max,0} (1 - D_C)$$

$$\Delta D_C = \max \left\{ 0, \frac{|\dot{\Delta}_n|}{\delta_\Sigma} \left[ \frac{T_n}{\sigma_{\max}} - \frac{\sigma_f}{\sigma_{\max,0}} \right] H(\Delta_{n,acc} - \delta_0) \right\}$$

$$\Delta_{n,acc} = \int_t |\dot{\Delta}_n| dt$$

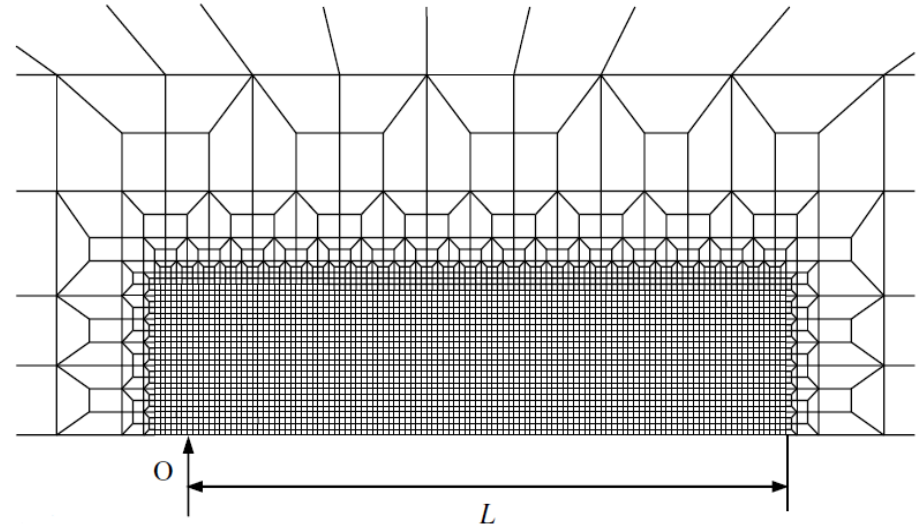
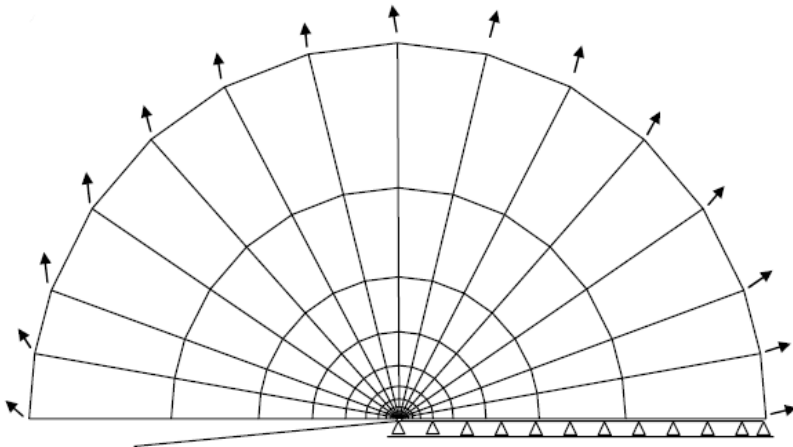
$$D_C = D_C + \Delta D_C$$

$$\left( \frac{J}{2\sigma_0} / \Lambda \right), (b / \Lambda), \left( \frac{j}{2\sigma_y} / \dot{\epsilon}_0 \Lambda \right), (\delta / \Lambda)$$

# PROGRESS

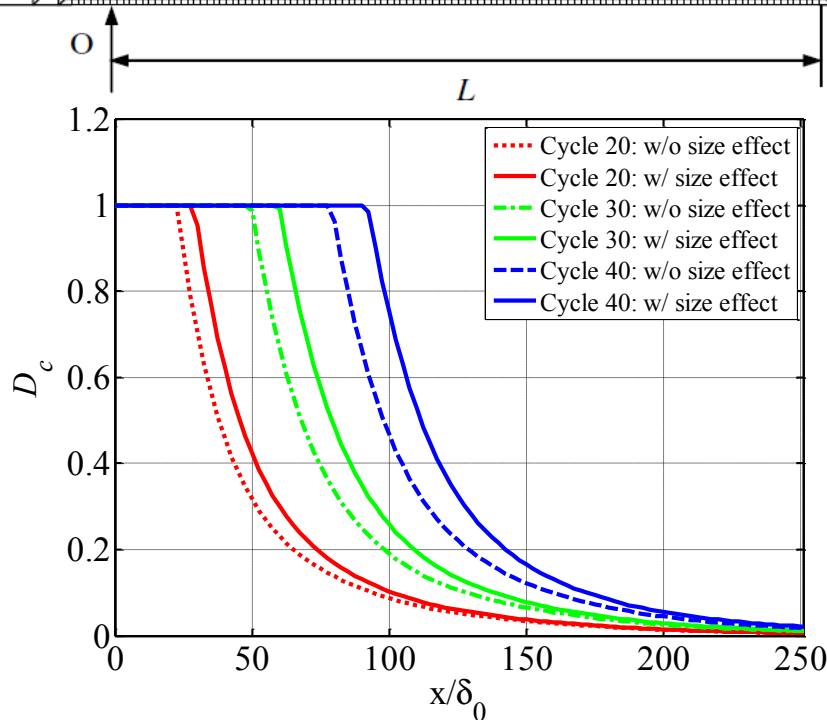
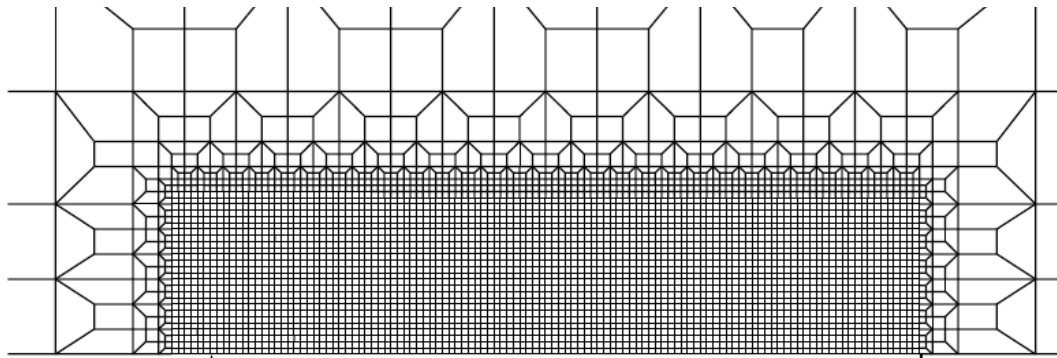
## Modified Boundary Layer Model

$$u_x(t) = K_I(t) \sqrt{\frac{r}{2\pi}} \frac{1+\nu}{E} (3-4\nu - \cos\theta) \cos\frac{\theta}{2}$$
$$u_y(t) = K_I(t) \sqrt{\frac{r}{2\pi}} \frac{1+\nu}{E} (3-4\nu - \cos\theta) \sin\frac{\theta}{2}$$
$$K(t) = \sqrt{\frac{EG(t)}{(1-\nu^2)}}$$



# PROGRESS

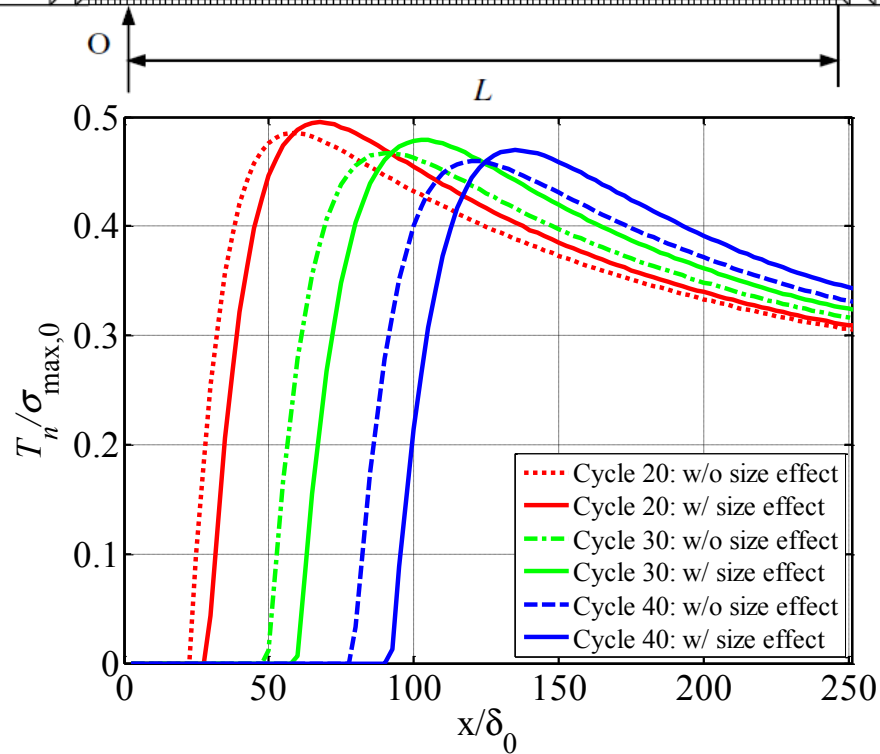
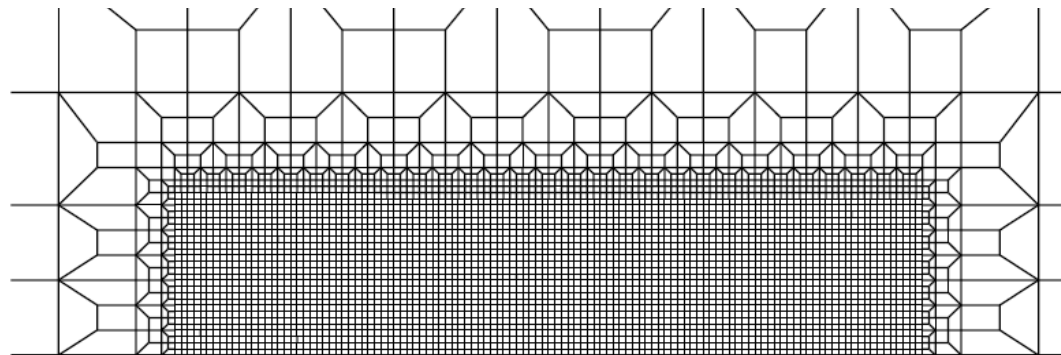
## Strain Gradients and FCG



- FCG Rates with SGP are larger than without

# PROGRESS

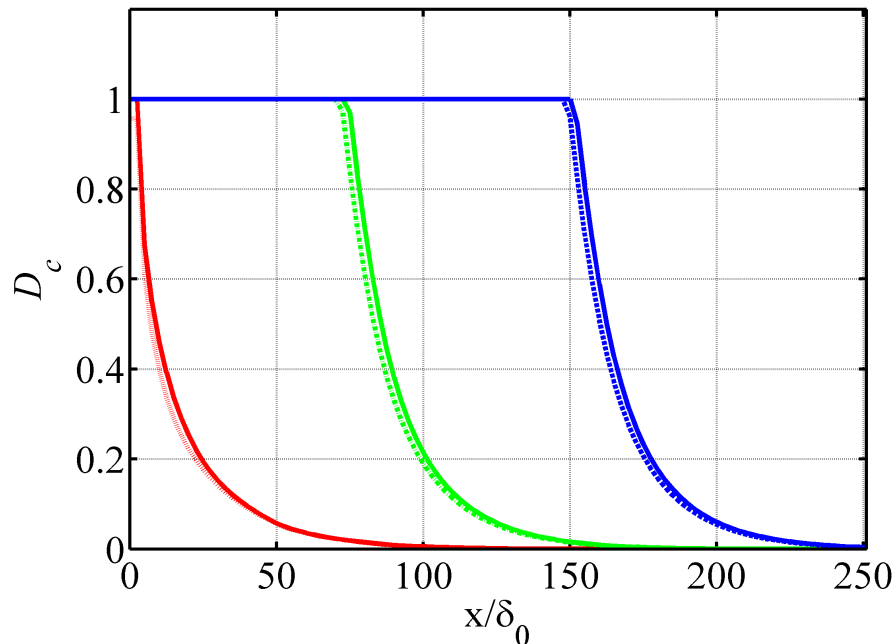
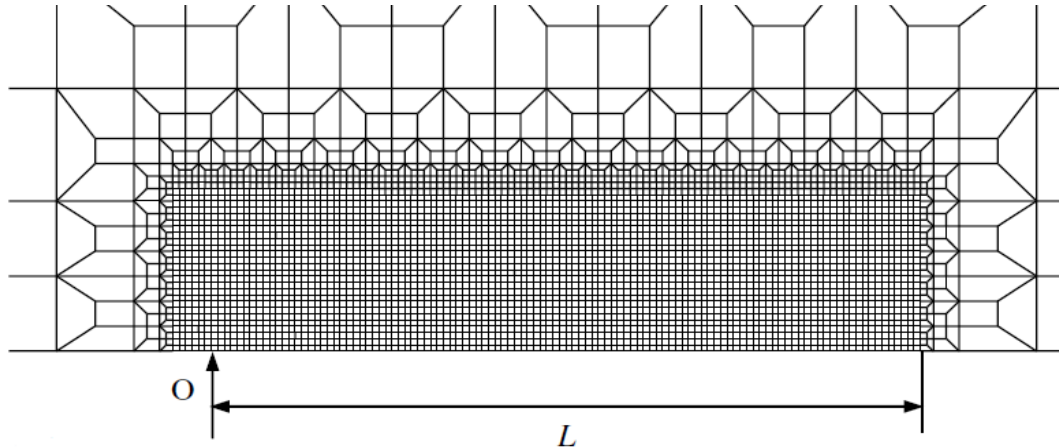
## Strain Gradients and FCG



- Opening stresses with SGP are larger than without

# PROGRESS

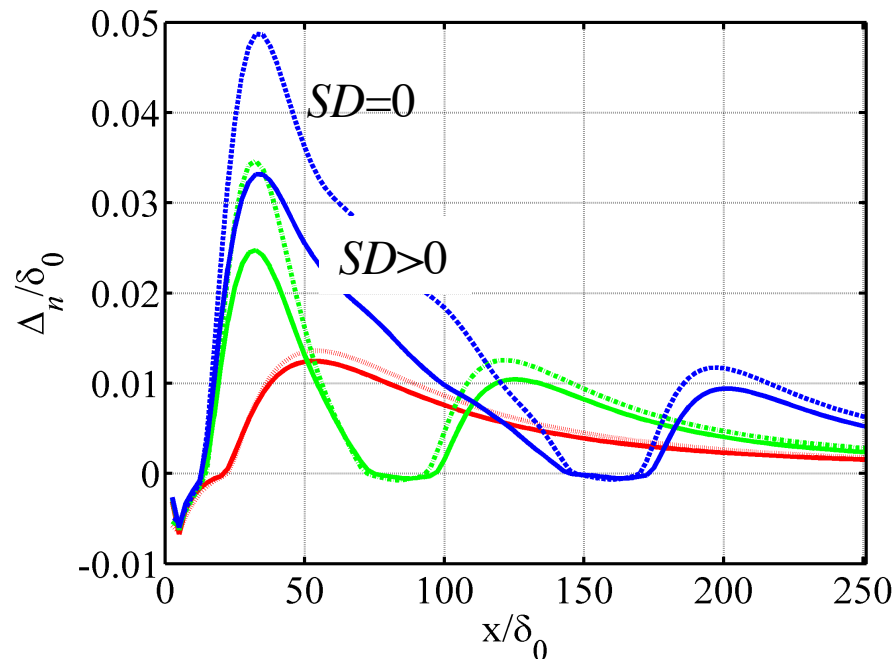
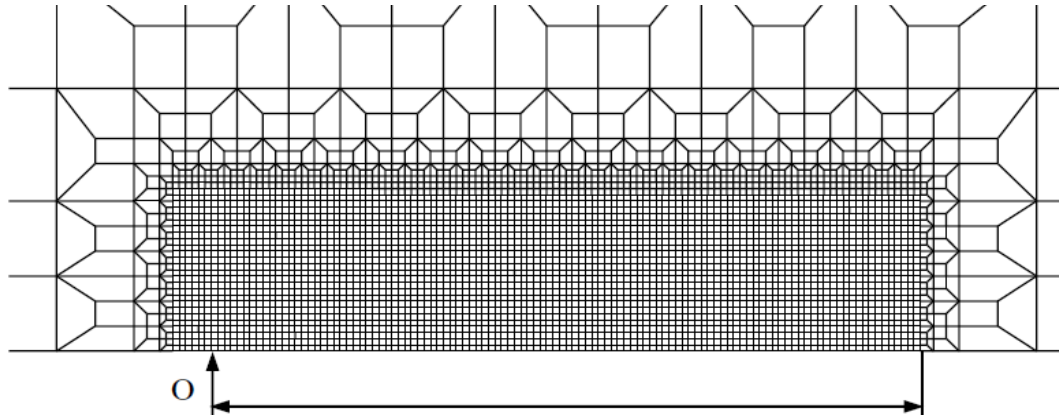
## Strength Differential and FCG



- FCG Rates appear as little affected by SD alone

# PROGRESS

## Strength Differential and FCG



- Crack closure appear as affected by SD alone



# TRAINING

## Computational Fracture Mechanics

Full semester course  
Online

<https://engineering.purdue.edu/ProEd/>

# CONCLUSION

- **Procured and characterized materials**
- **Established interaction with Jeff Hawk, NETL Albany**
- **Property measurements are forthcoming**
- **Computational mechanics: Advanced model implementation on several fronts**
  - Strain gradients raise the open stress level and appear to accelerate crack growth
  - Strength differential alters the crack closure conditions but appears to not accelerate crack growth
- **Mechanics indicates the SGP and SD effects alter the crack tip stress state which would alter crack growth in creep and environmental degradation**