

Microstructure-focused Durability and Damage Tolerance Research at NASA Langley

Jacob Hochhalter ...Continuum modeling

Vipul Gupta ...Microscopy

William Leser ...SMA experiments

Stephen Cornell ...Summer student

Andy Newman ...Fatigue experiments

Terryl Wallace ...Material science

Vesselin Yamakov ...Molecular dynamics

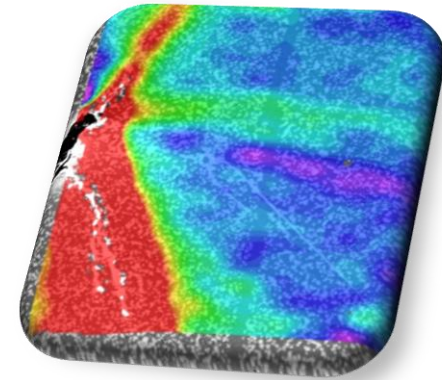
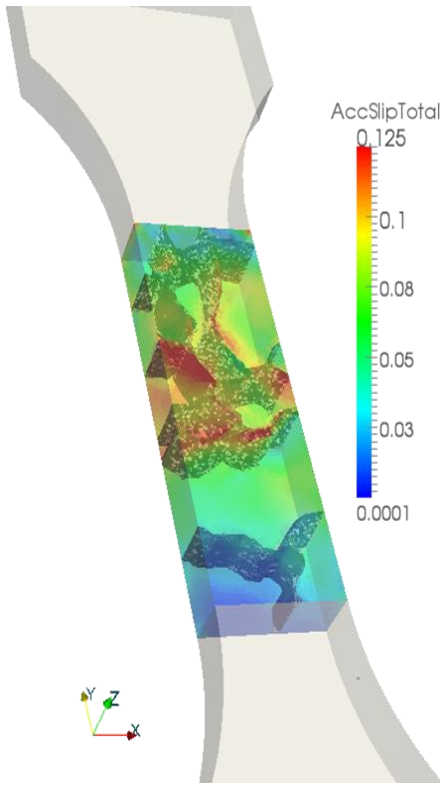
Ed Glaessgen ...Management

Steve Smith ...Management

NASA Langley Research Center, Hampton, VA

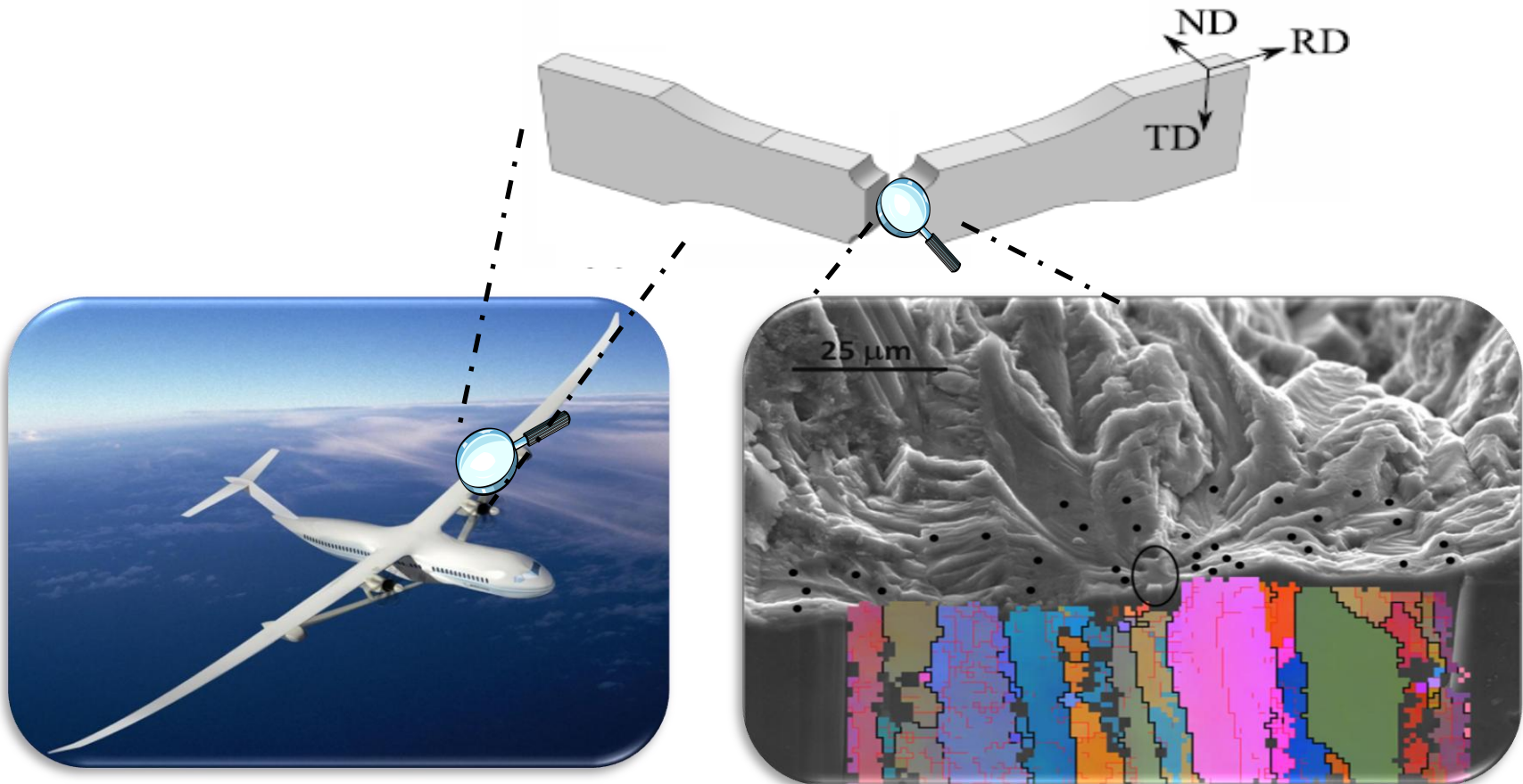
National Institute of Aerospace, Hampton, VA

Texas A&M, College Station, TX



Our objective

To better understand and prognose the distribution of fatigue behavior as it relates to inherent material inhomogeneities.



Something we know

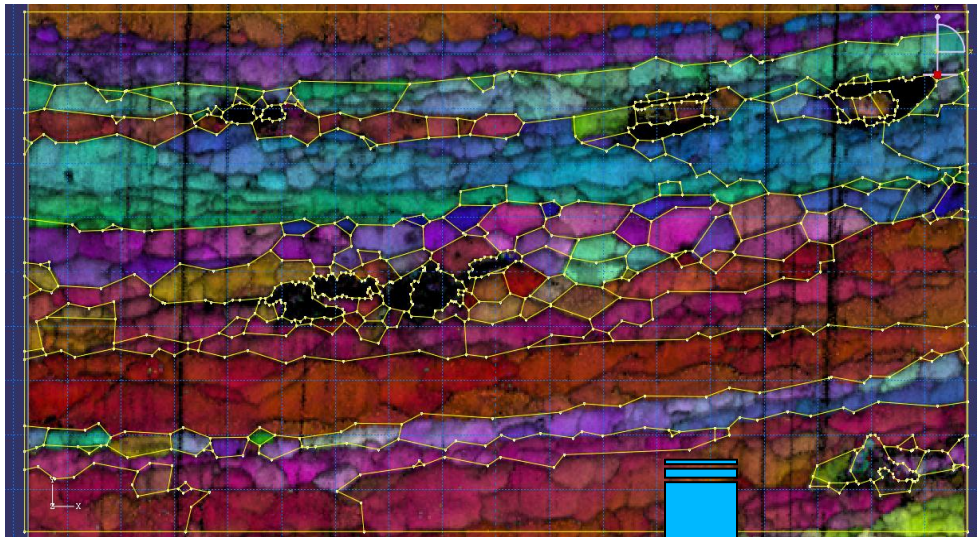
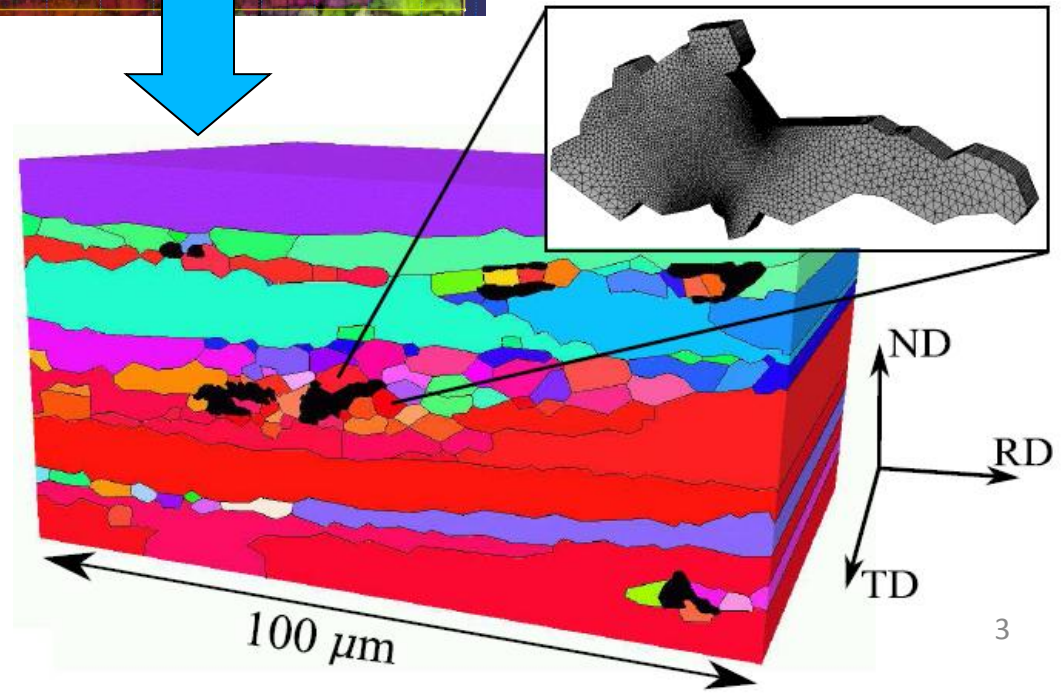


Photo courtesy Northrup
Grumman Corp.

Modeling engineering alloys in
3D is **complex**

How can we study one
question at a time?
...
and how can we eventually
answer time-sensitive
questions using high-fidelity
approaches?



Outline

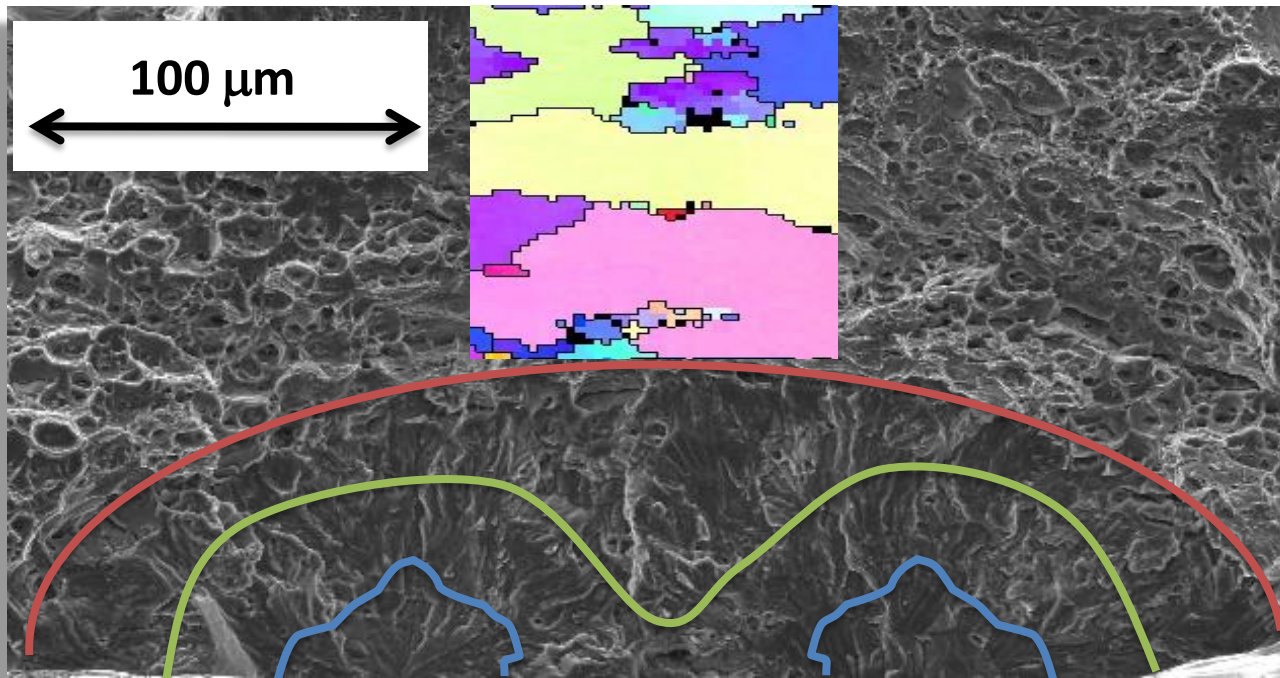


- Brief branch portfolio (collaborations)
 - Ni superalloy
 - Crack locating
- Materials Genome Initiative (MGI)
 - Fabrication and testing of various Al-Cu alloys
- Airframe Digital Twin (ADT)
 - Embedded shape memory alloy particles as crack detection sensors

Ni Superalloy: Proposed Question



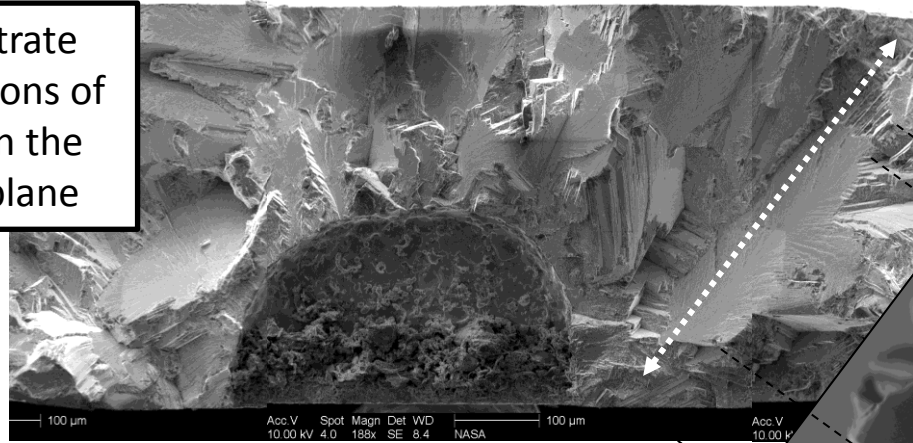
Can we predict life for fatigue critical components that are just a grain or two thick?



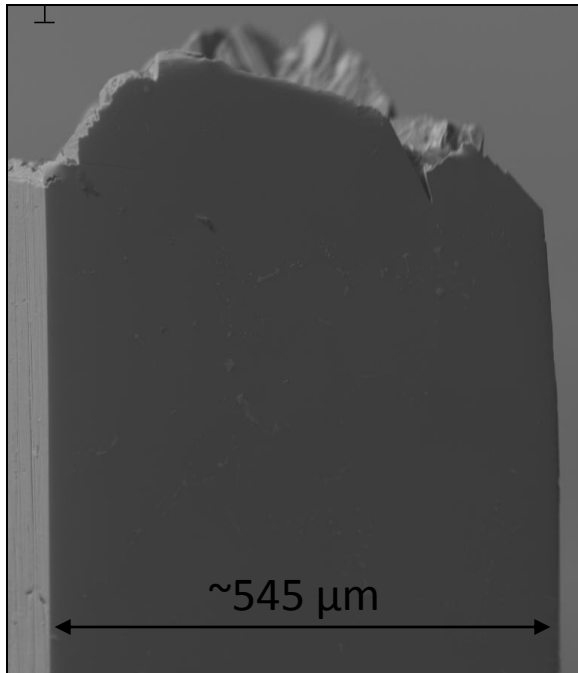
Existing modeling approaches failed to predict fatigue life 70% of the time!

Ni Superalloy: Initiation

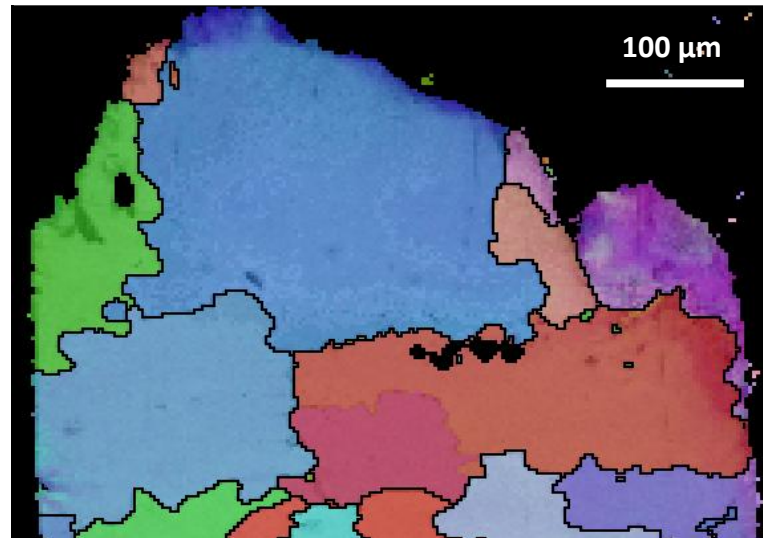
Broken lines illustrate approximate locations of grains/features on the cross-sectioned plane



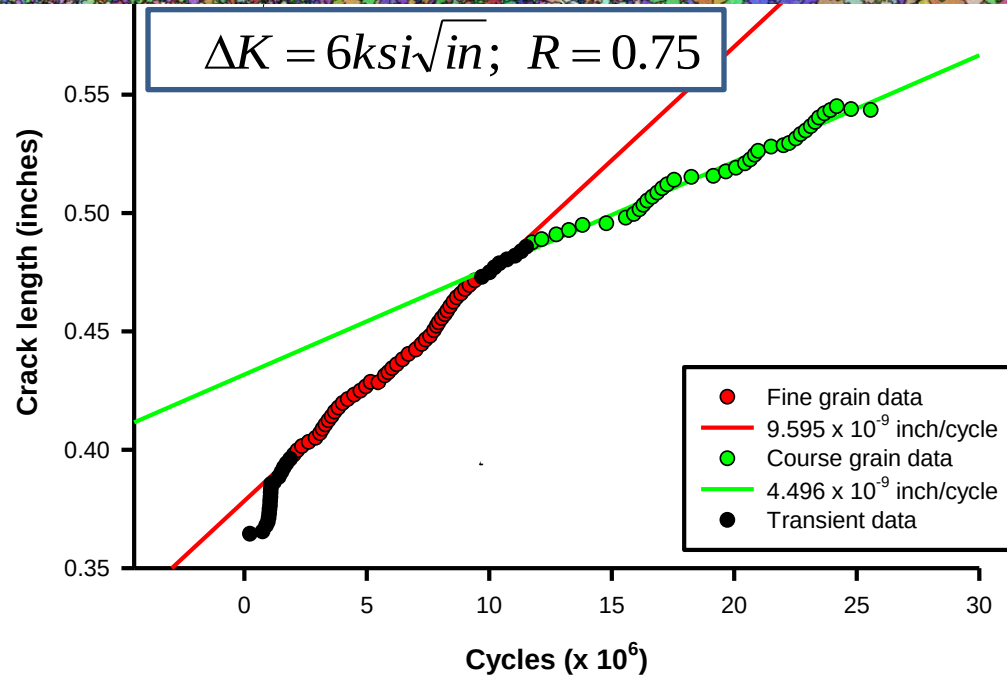
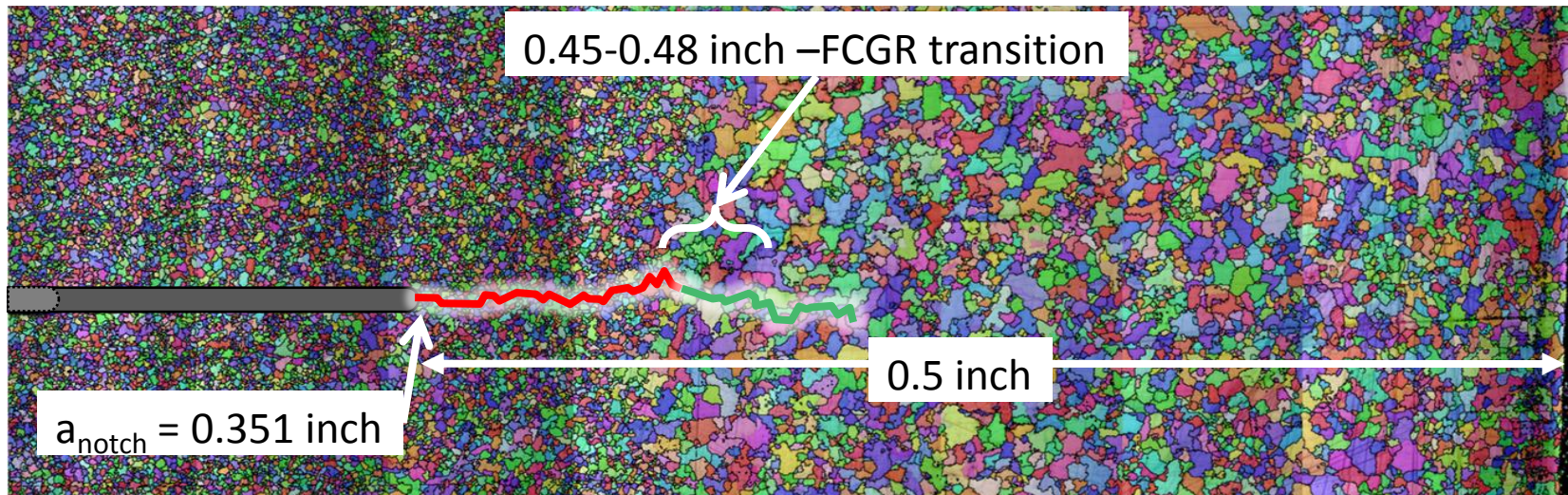
SEM image



EBSD Orientation Map

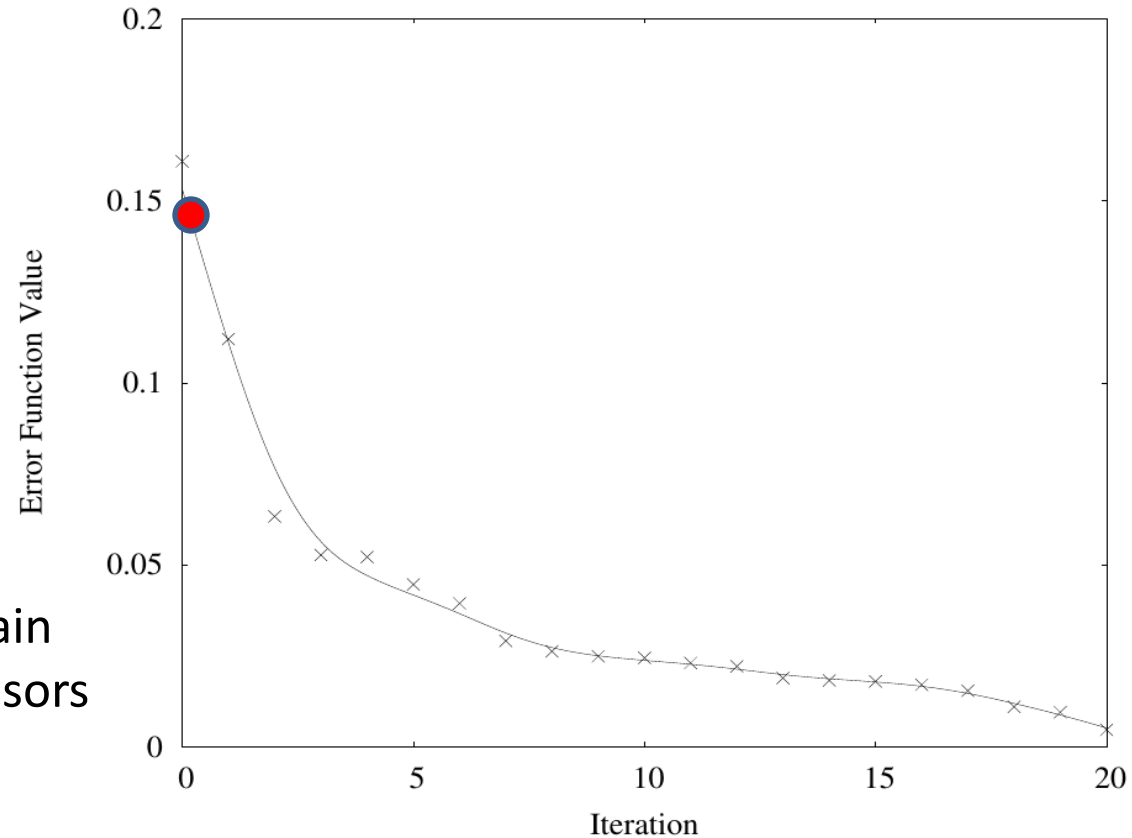
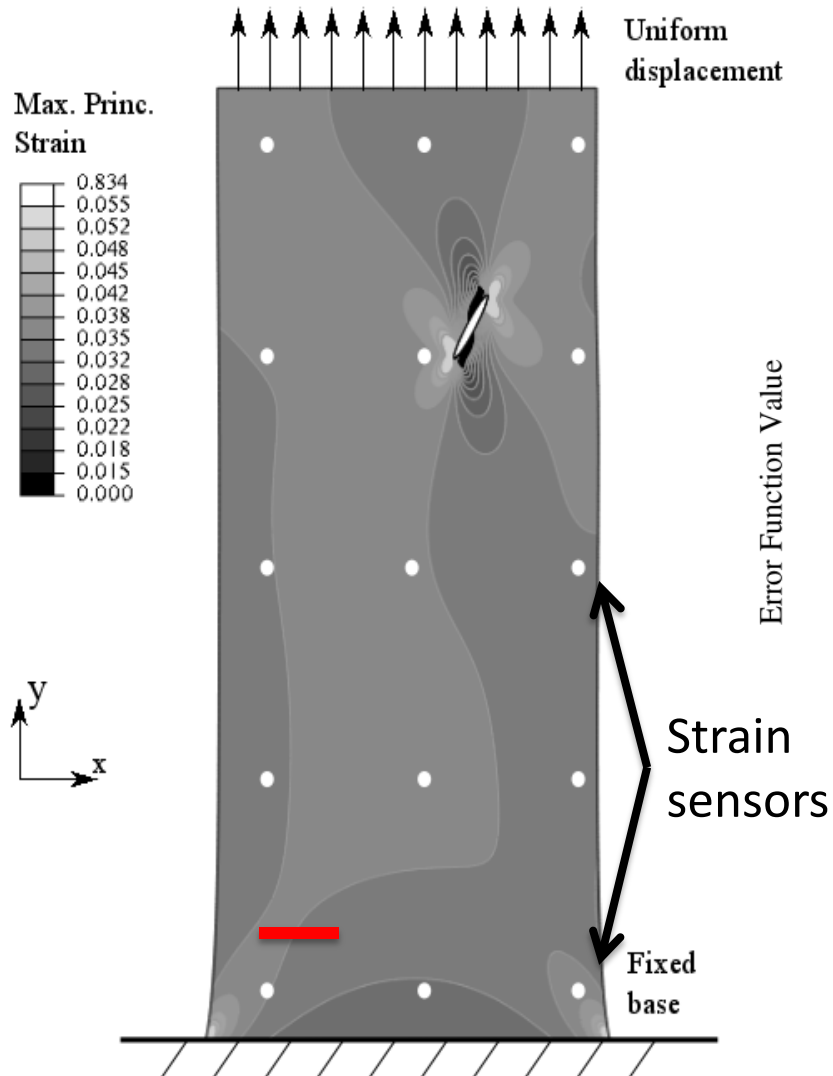


Ni Superalloy: Propagation



Apparent 2x decrease in crack growth rates around $a = 0.48$ inch.

Crack Locating Study



Outline



- Brief branch portfolio (collaborations)
 - Ni superalloy
 - Crack locating
- Materials Genome Initiative (MGI)
 - Fabrication and testing of various Al-Cu alloys
- Airframe Digital Twin (ADT)
 - Embedded shape memory alloy particles as crack detection sensors

THE U.S. MATERIALS GENOME INITIATIVE

"...to discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative"
— President Obama, 2011

Meeting Societal Needs

Advanced materials are at the heart of innovation, economic opportunities, and global competitiveness. They are the foundation for new capabilities, tools, and technologies that meet urgent societal needs including clean energy, human welfare, and national security.



Clean Energy

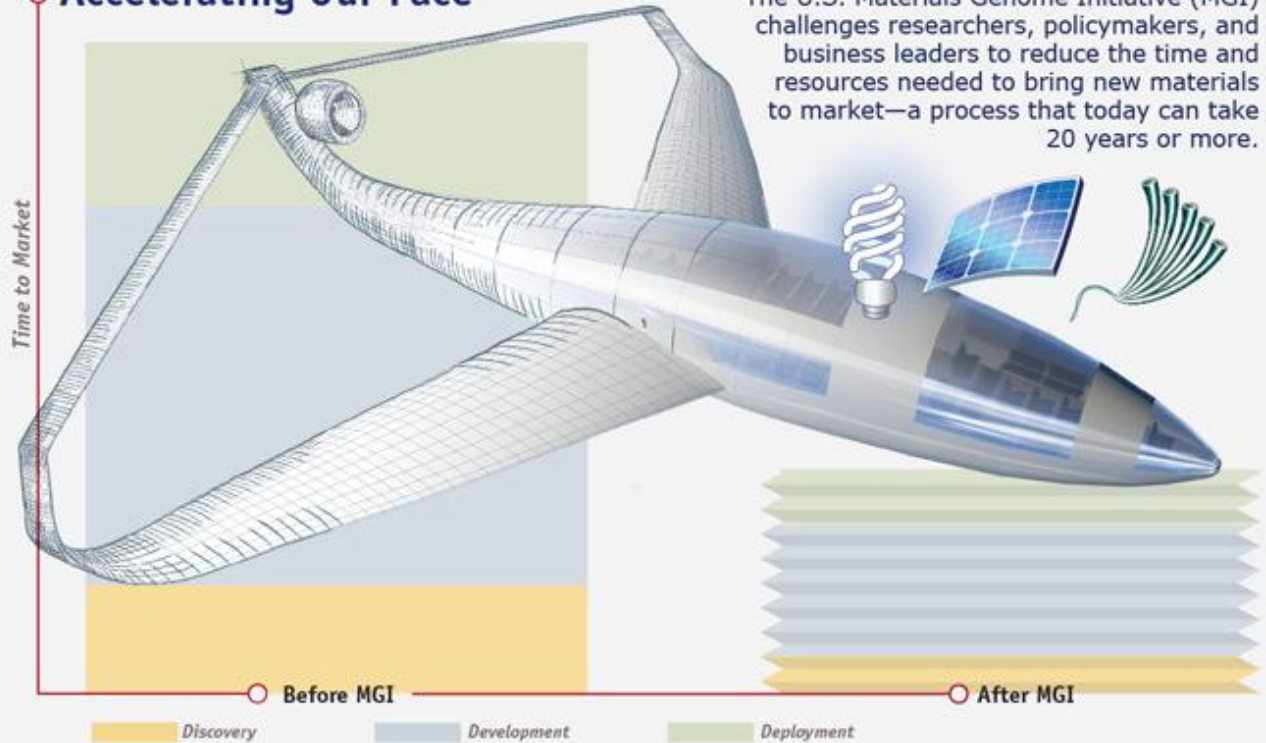


Human Welfare



National Security

Accelerating Our Pace



Building Infrastructure for Success

The MGI is a multi-agency initiative to renew investments in infrastructure designed for performance, and to foster a more open, collaborative approach to developing advanced materials, helping U.S. Institutions accelerate their time-to-market.



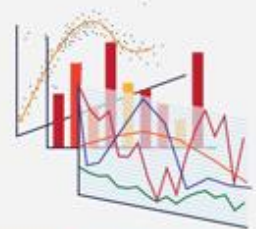
Computational tools



Experimental tools

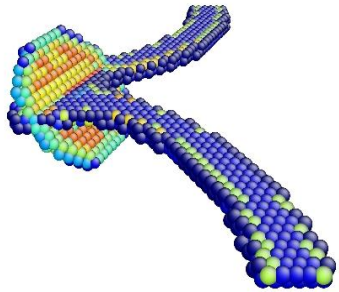


Collaborative networks



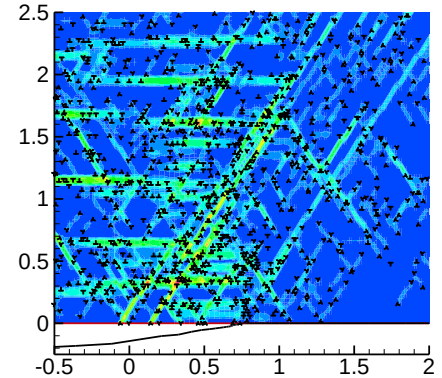
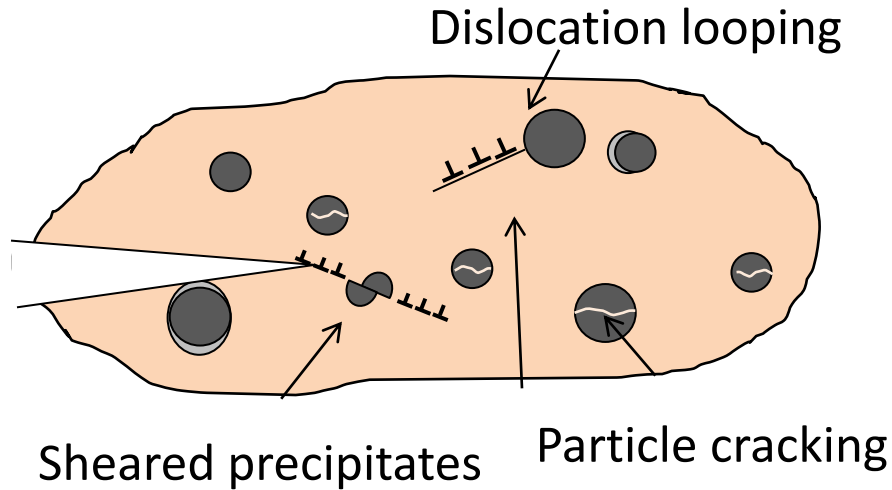
Digital data

Studying Fundamental Mechanisms



Dislocation-Precipitate Interaction

Warner et al.

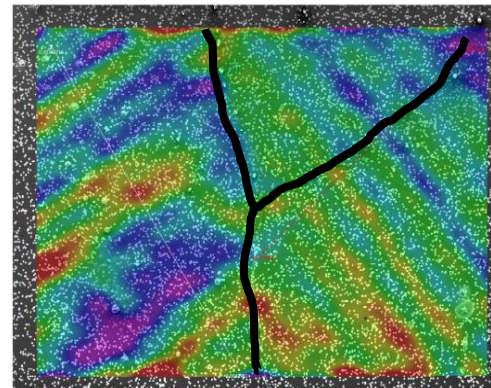
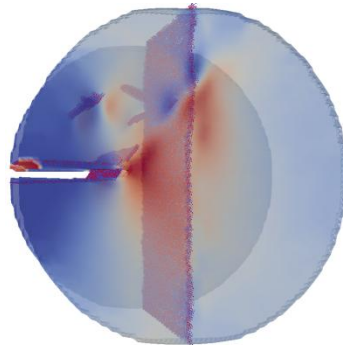


Dislocation-Crack Interaction

Curtin et al.

Crack-Grain Boundary Interaction

Yamakov et al.

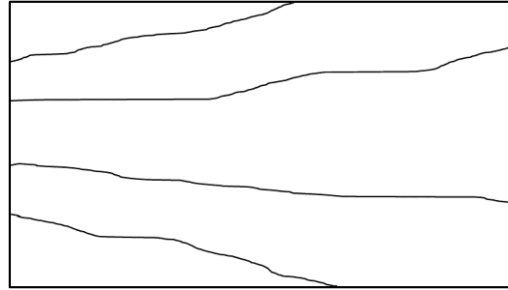
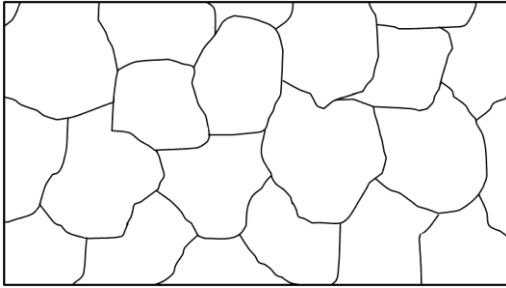


In-situ Digital Image Correlation

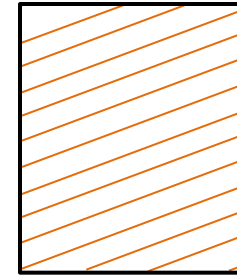
Gupta et al.

Al-Cu Fabrication

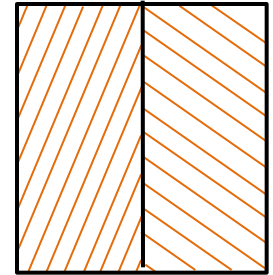
Polycrystal



Single crystal



Bi-crystal



Vacuum induction melter



Bridgman furnace



Single crystal
crucible



Bi-crystal
crucible

Al-Cu Crystal Plasticity Models

Multiplicative decomposition

$$F = F^e F^p F$$

Precipitation Hardness¹:

$$\dot{g}^\alpha = G_o \left(\frac{g_o - g^\alpha}{g_s - g_o} \right) H^{\alpha\beta} |\dot{\gamma}^\beta|$$

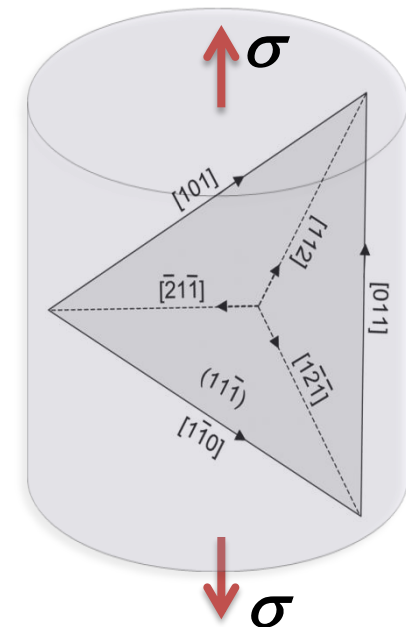
Grain-size-dependent Hardness²:

$$\dot{g} = G_o \left(\frac{g_s - g}{g_s - g_o} \right) \sum_\alpha |\dot{\gamma}^\alpha| + \frac{k_o a^2 \mu^b}{2(g - g_o)} \sum_\alpha \lambda^\alpha |\dot{\gamma}^\alpha|$$

Several parameters to calibrate

Slip rule:

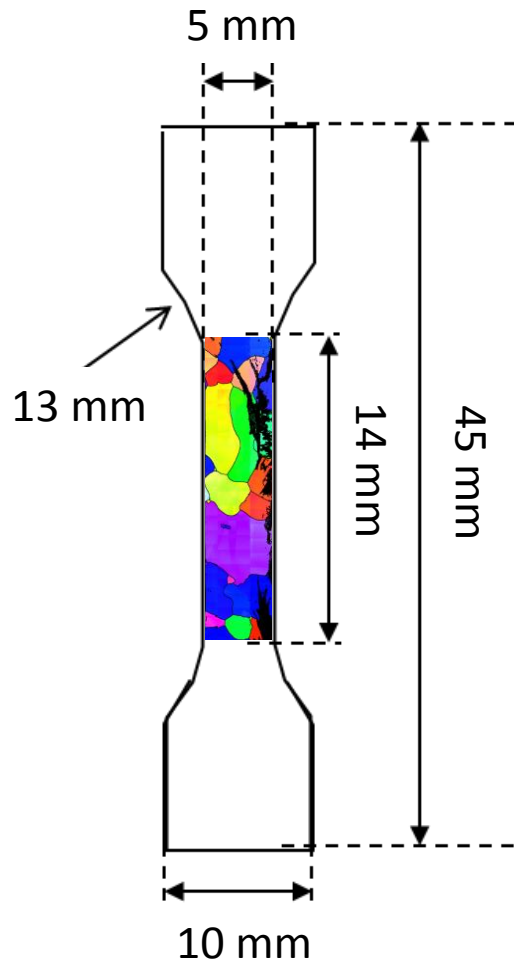
$$\dot{\gamma}^\alpha = \dot{\gamma}_o \frac{\tau^\alpha}{g_\alpha} \left| \frac{\tau^\alpha}{g_\alpha} \right|^{\frac{1}{m}-1}$$



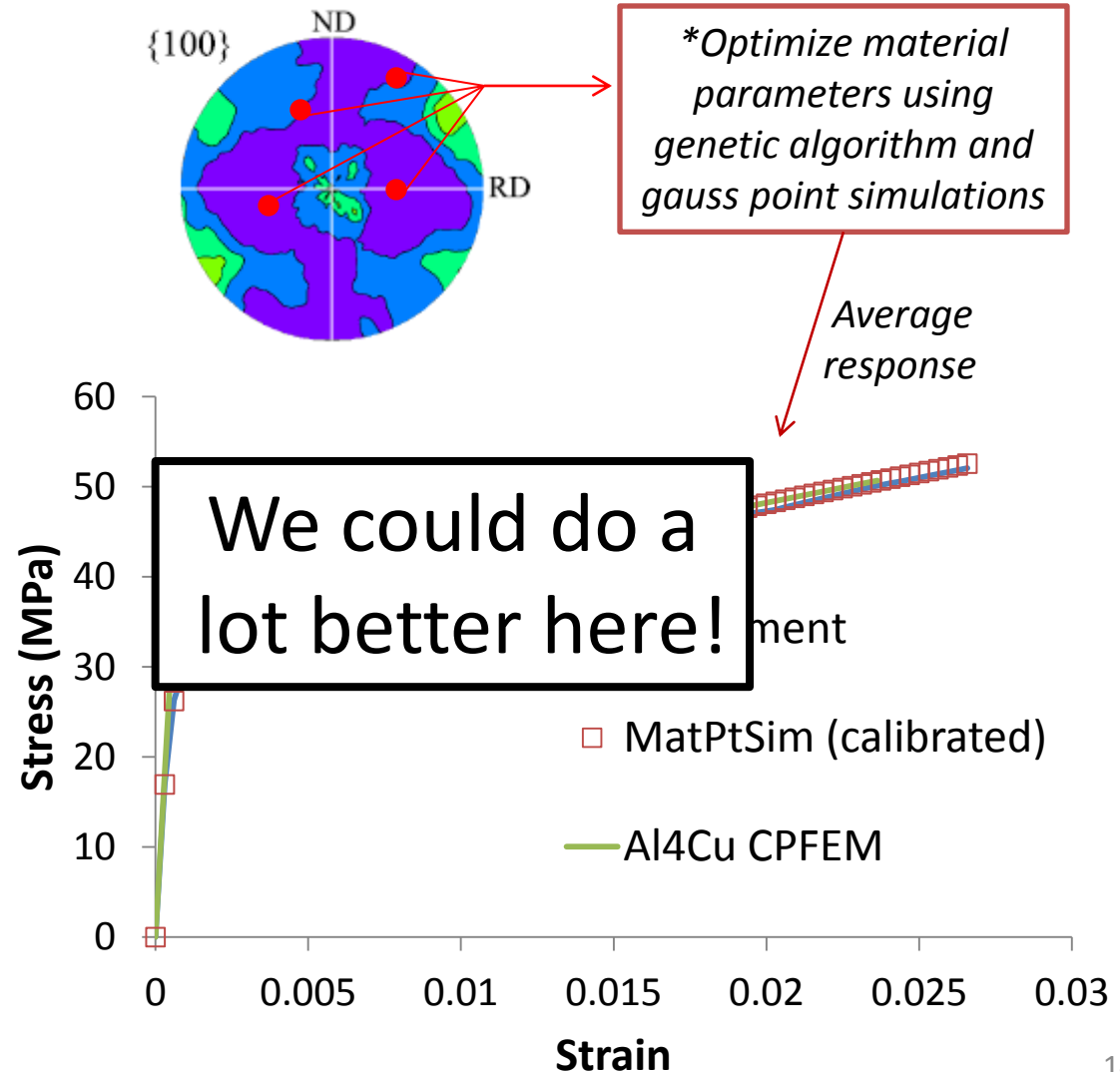
Al-Cu Material Model Calibration



Experiment, Uniaxial Tension



Material Point Simulations



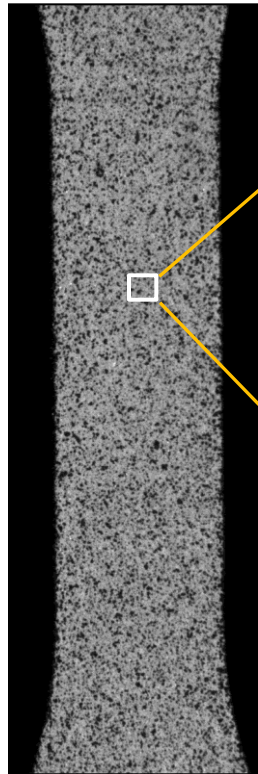
*Measured nominal stress-strain used as target in genetic algorithm fit of material parameters

Full-field Strains with Image Correlation

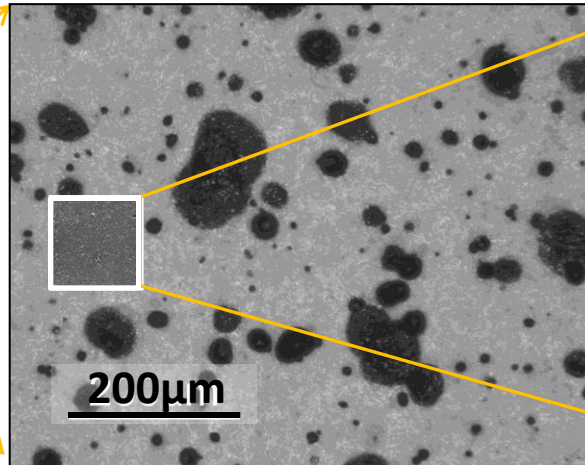


Optical image correlation

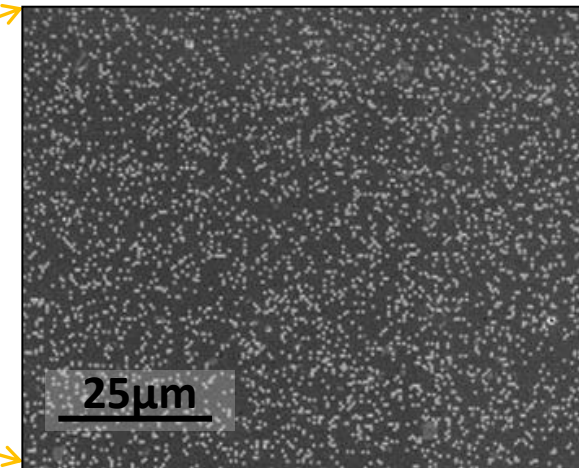
Secondary electron image correlation



5 mm



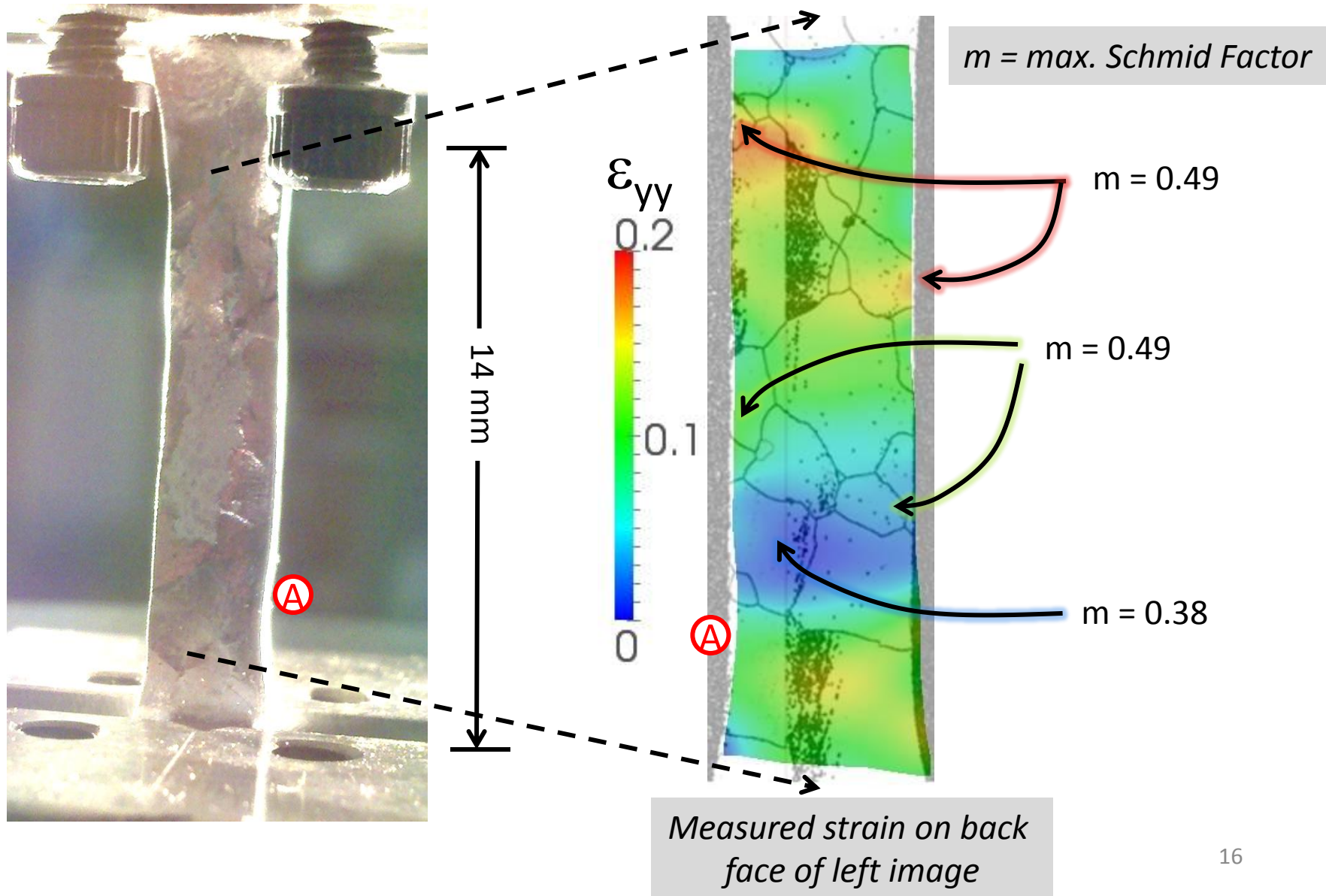
- Spray paint, air-brush
- Base element $\sim 25\text{-}150\ \mu\text{m}$
- Local “grain-to-grain” strain variation in addition to average deformation behavior
- Fatigue, fracture and deformation studies within larger regions



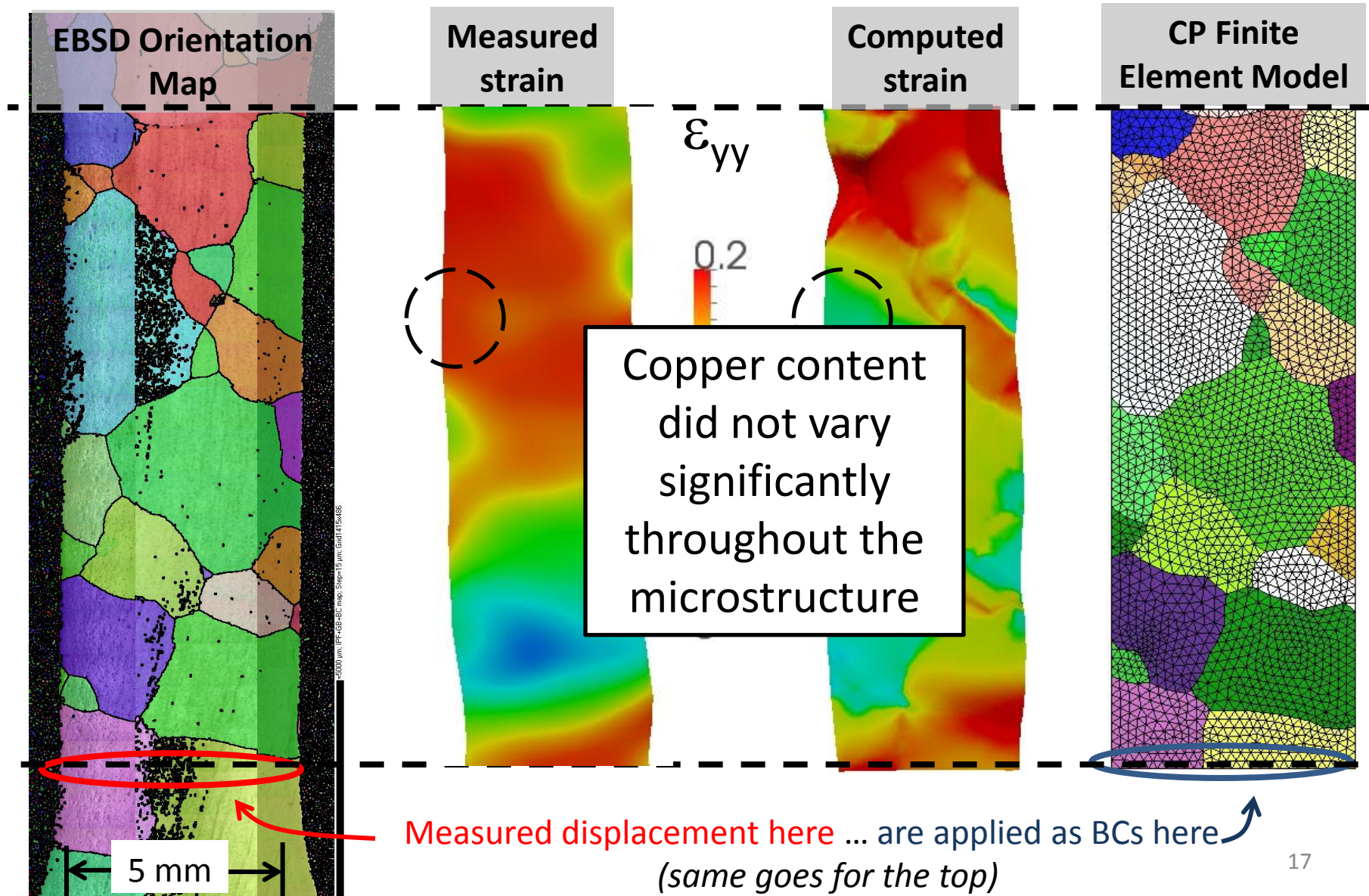
- E-beam lithography
- Base element $\sim 150\text{-}5000\ \text{nm}$
- Microstructural (grain boundaries, intermetallic particles, crack tip etc.) effects on strain fields
- Microstructurally sensitive cracking and deformation studies

3D Grain-scale Strain Measurement

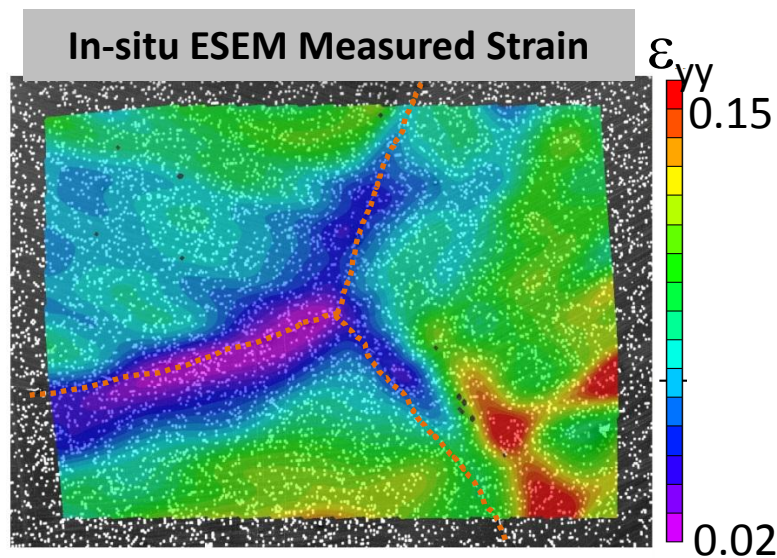
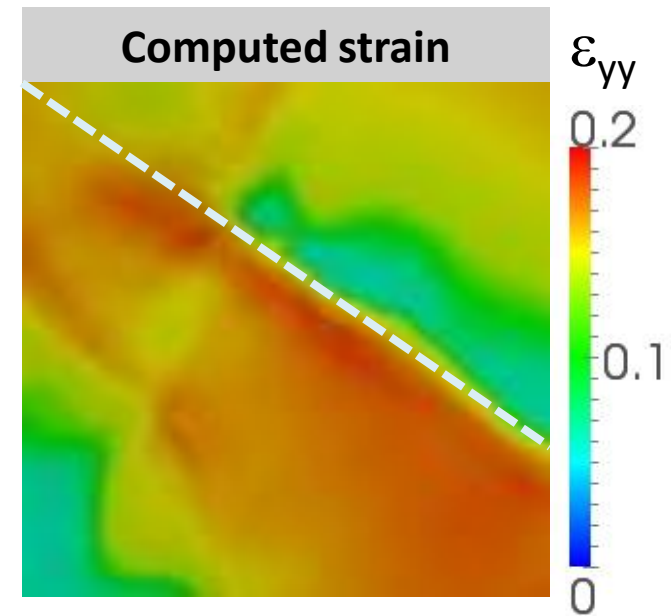
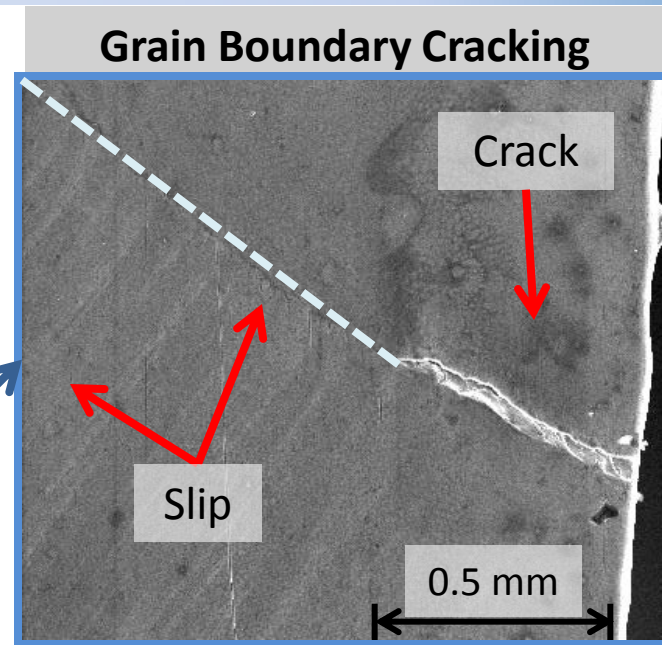
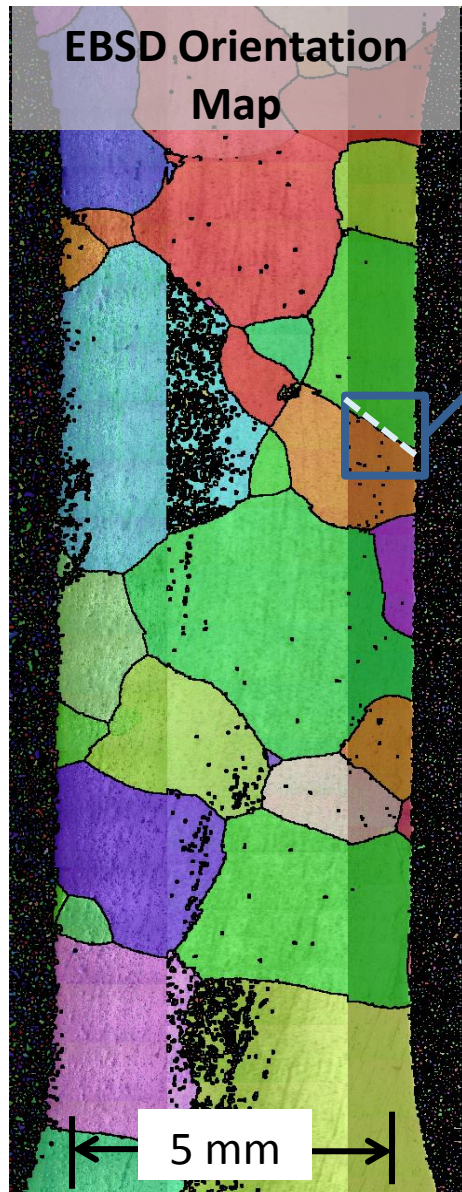
polycrystalline Al-4Cu



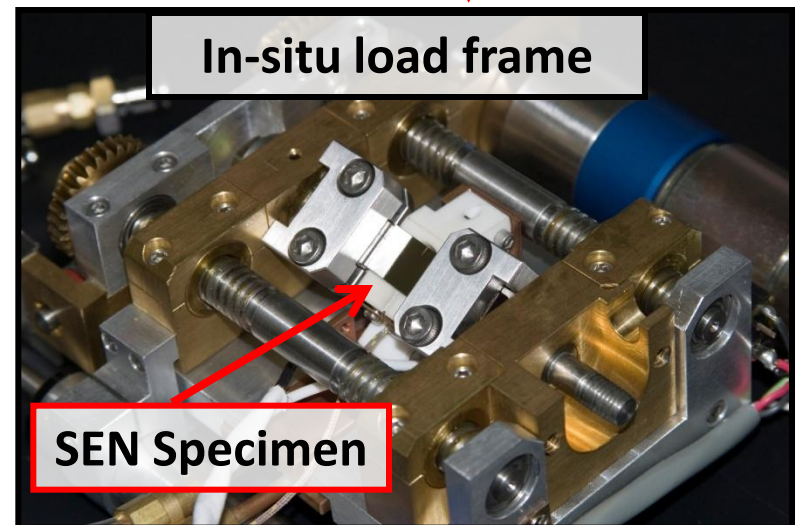
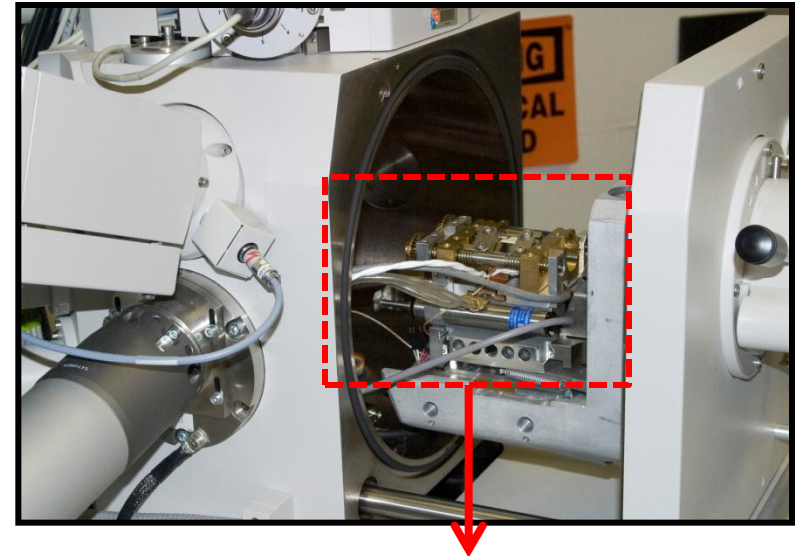
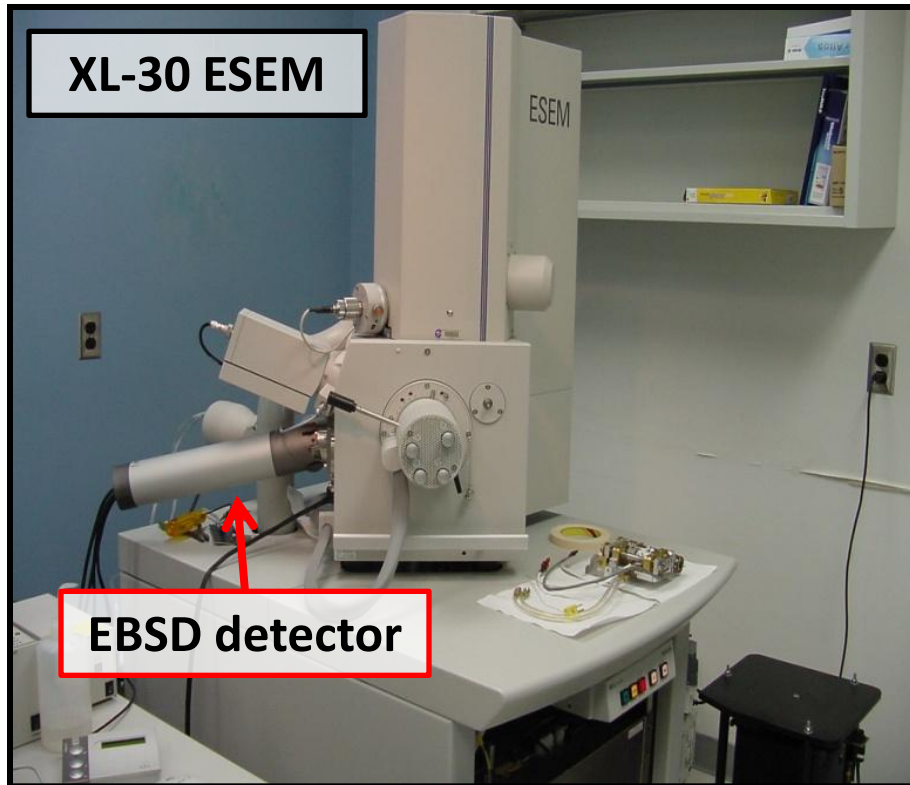
Grain-scale Results Comparison



Grain-scale Results Comparison



In-situ ESEM Strain Measurement *single crystal Al-2Cu*

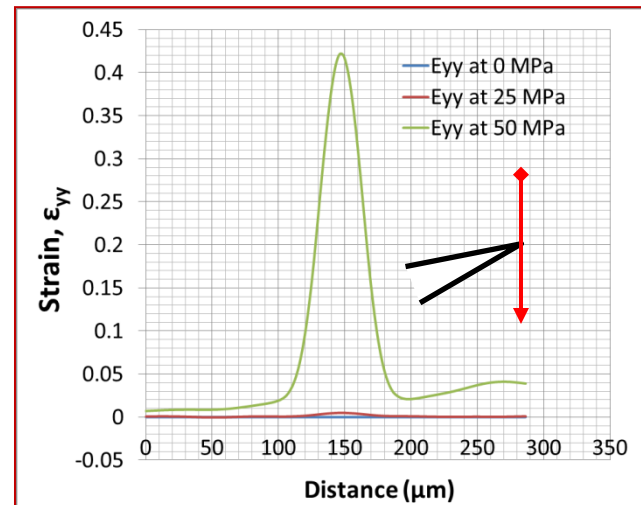
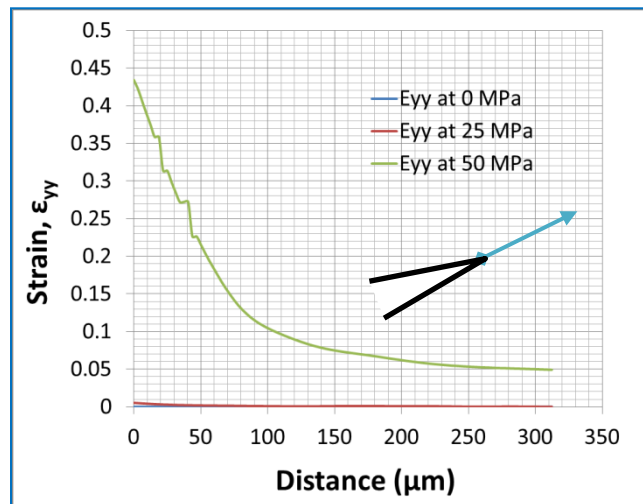
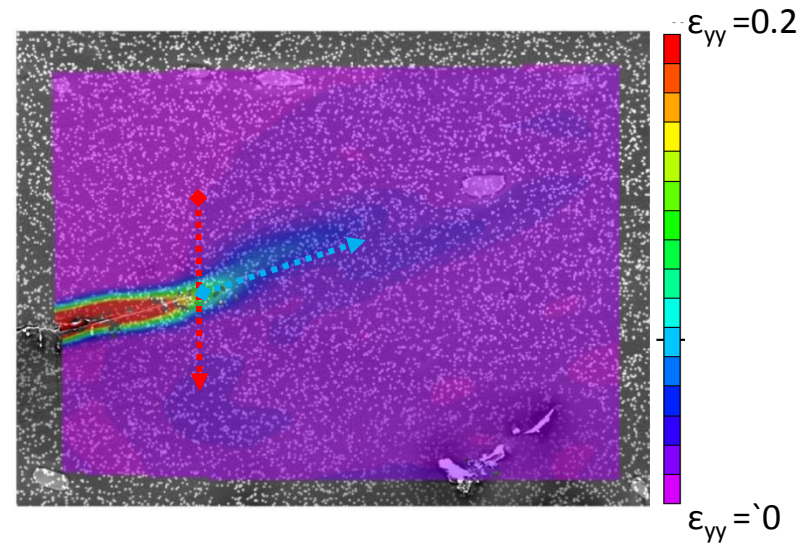
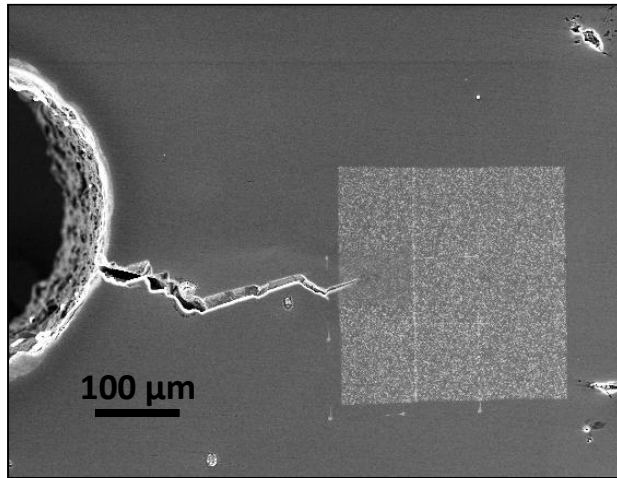


- Resolution < 2nm @ 7 Torr (FEG)
- Operating environment
High Vacuum to 20 torr (H_2O , N_2)
- Temp. -20 to +1000 °C
- Tensile Stage, 4 kN, up to 1 Hz

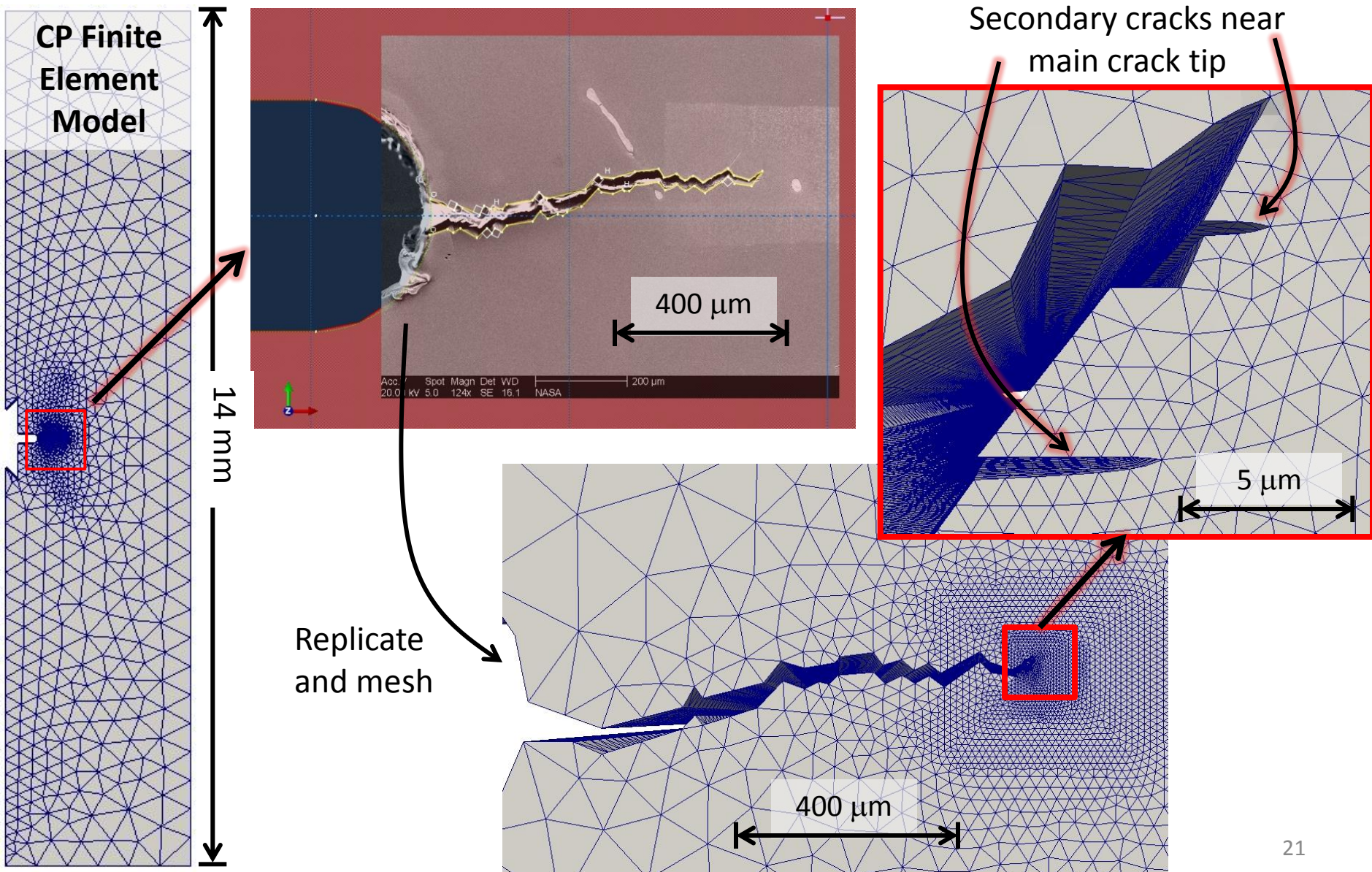
Crack Tip Strain Localization



Single crystal Al-2Cu



Detailed Replication of the Fatigue Precrack

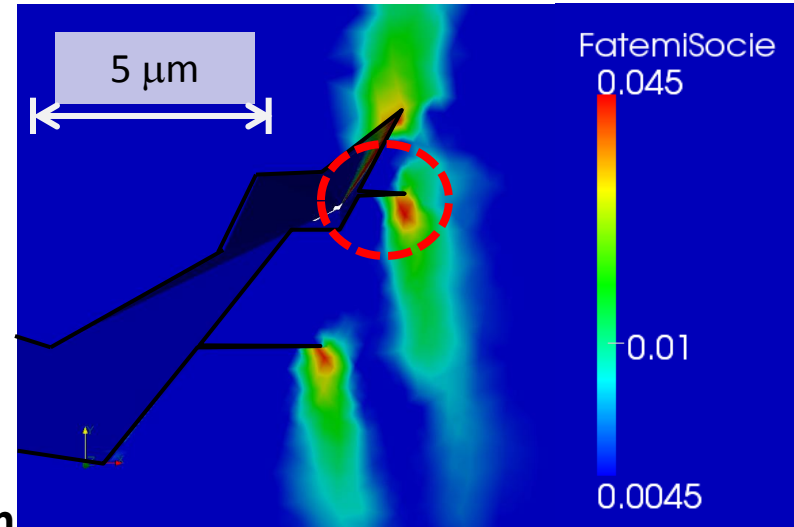
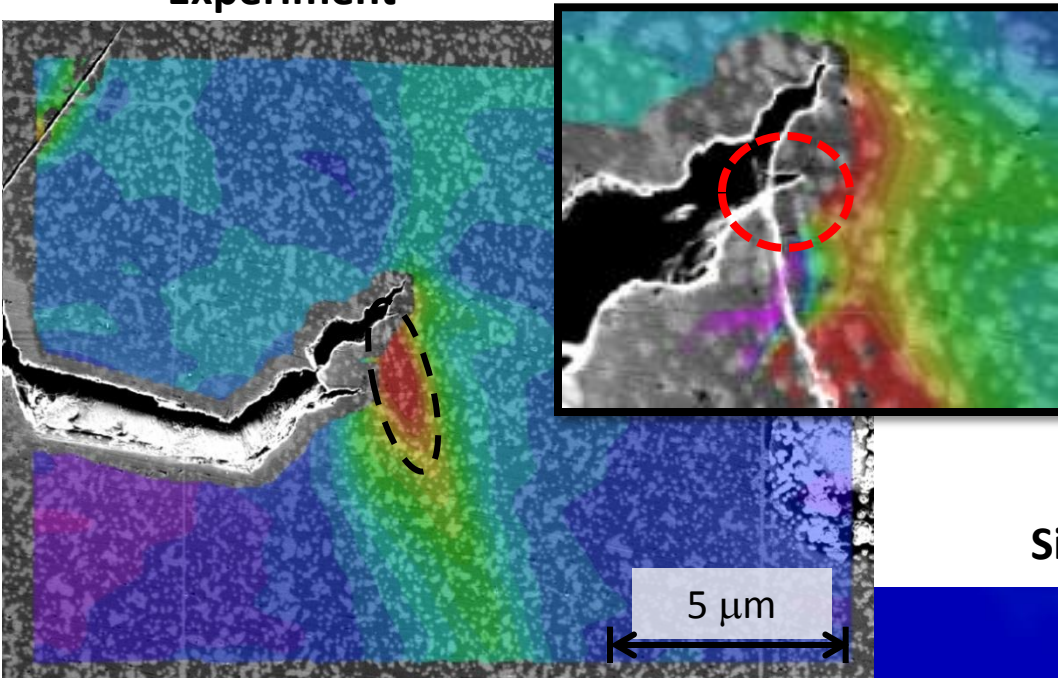


In-situ ESEM Results Comparison

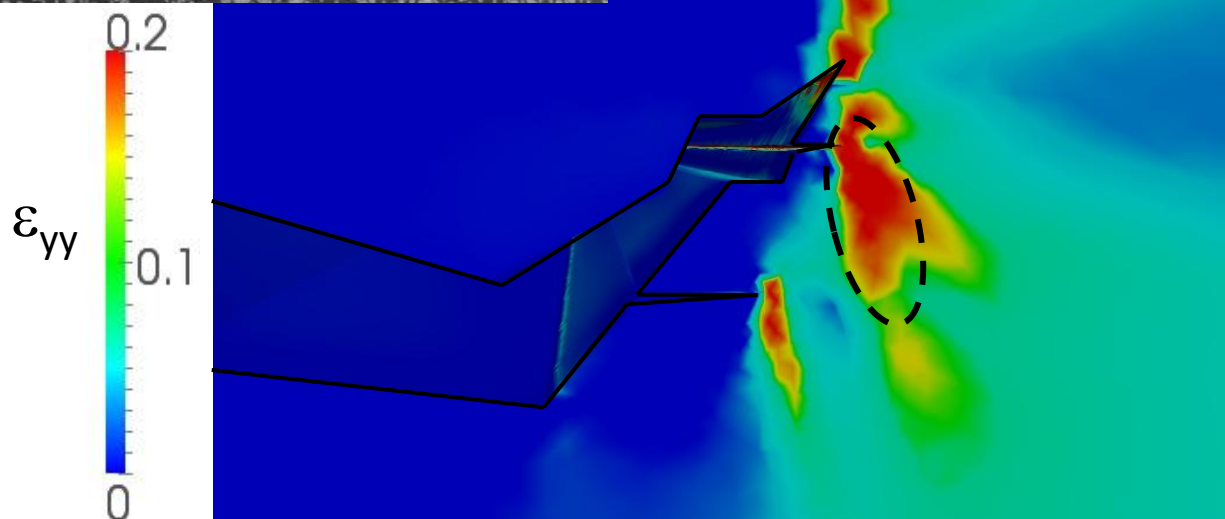
single crystal Al-2Cu



Experiment



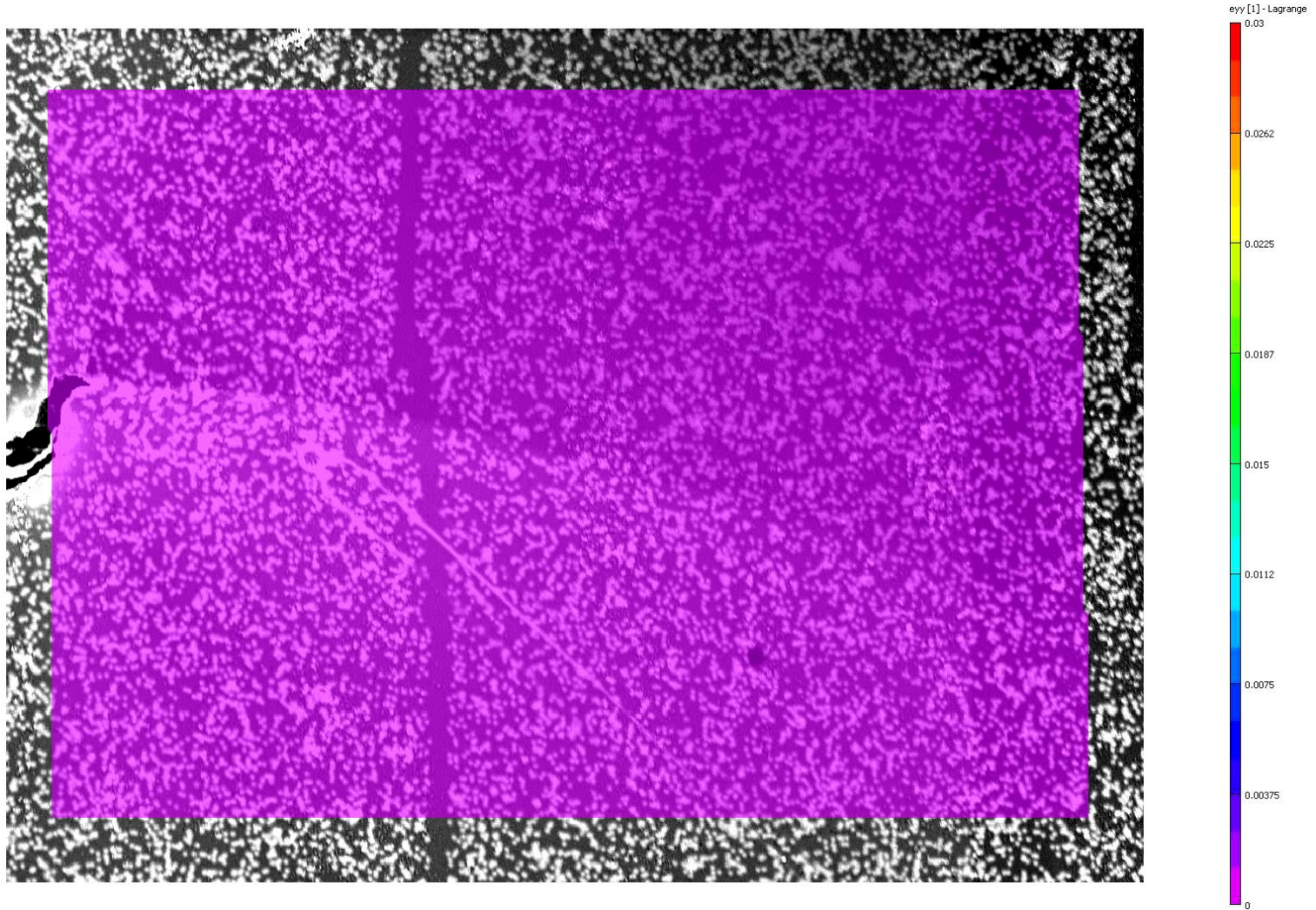
Simulation





In-situ ESEM Strain Accumulation Measurement *single crystal Al-2Cu*

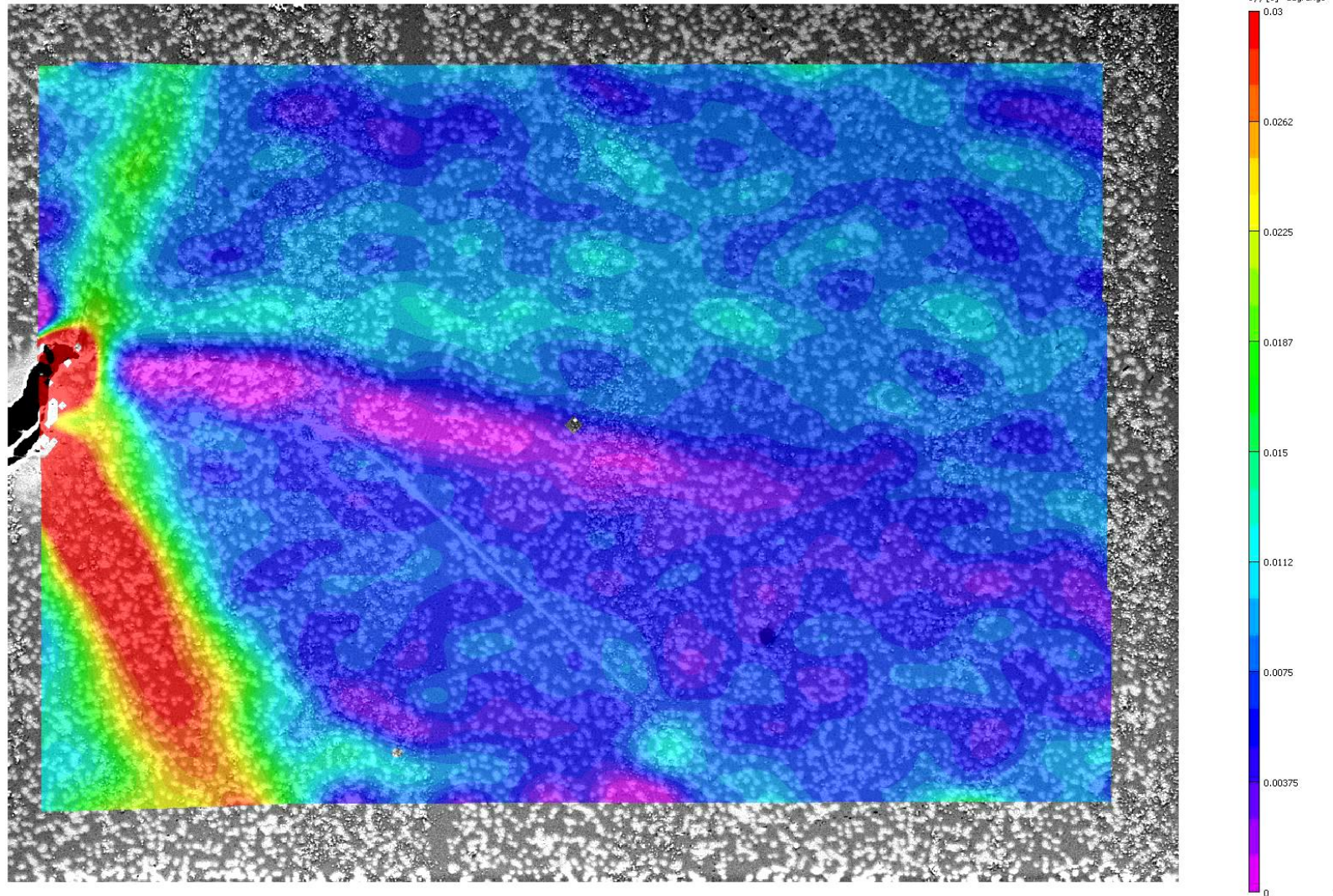
Cycle 1



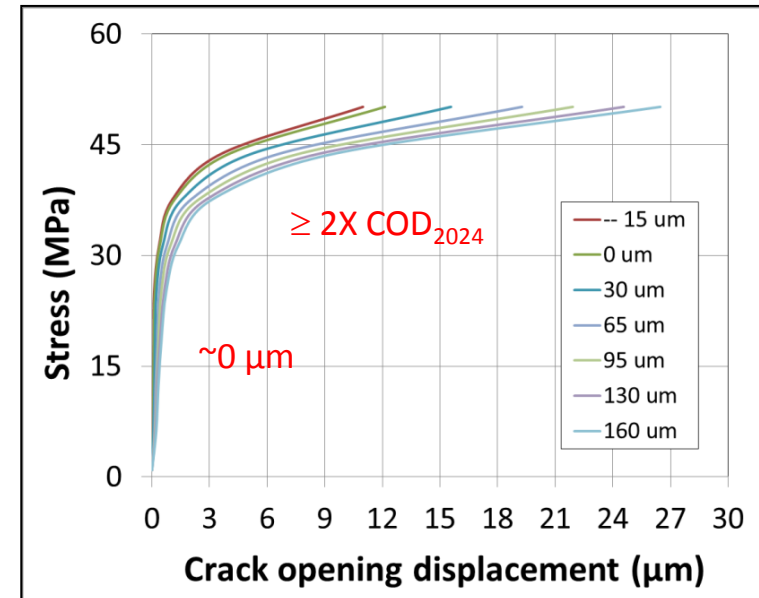
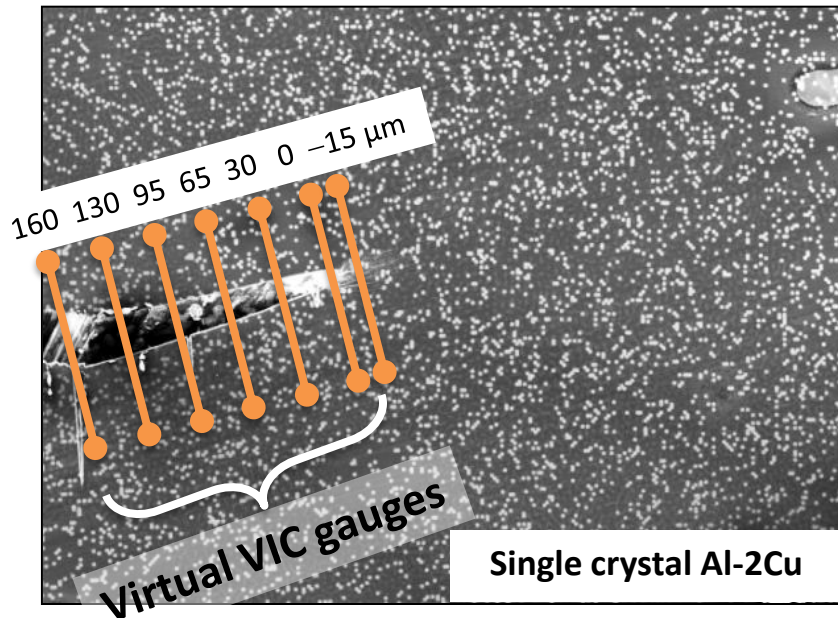
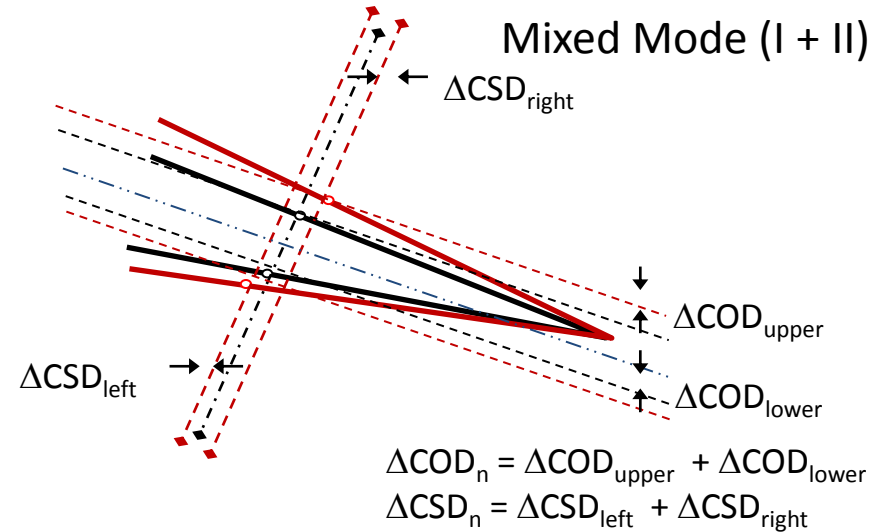
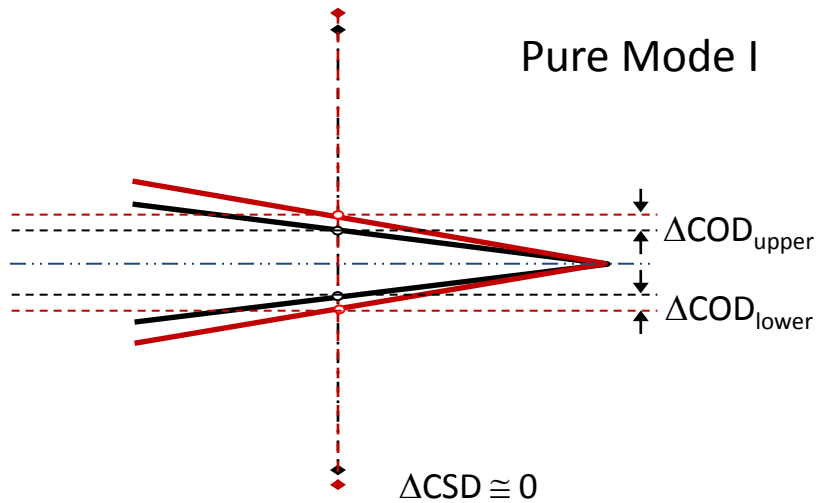
In-situ ESEM Strain Accumulation Measurement *single crystal Al-2Cu*



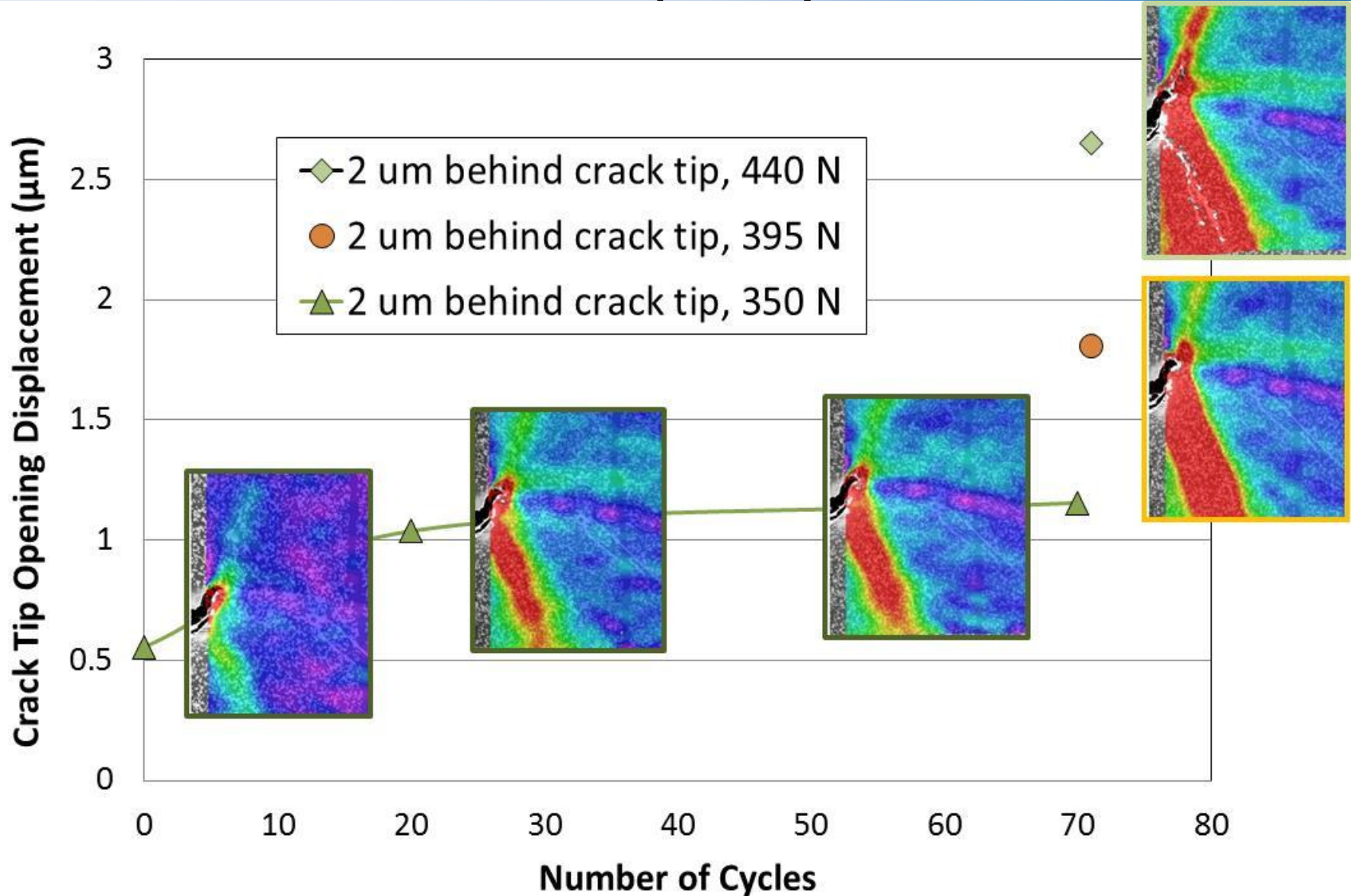
Cycle 72



Crack Opening Displacements

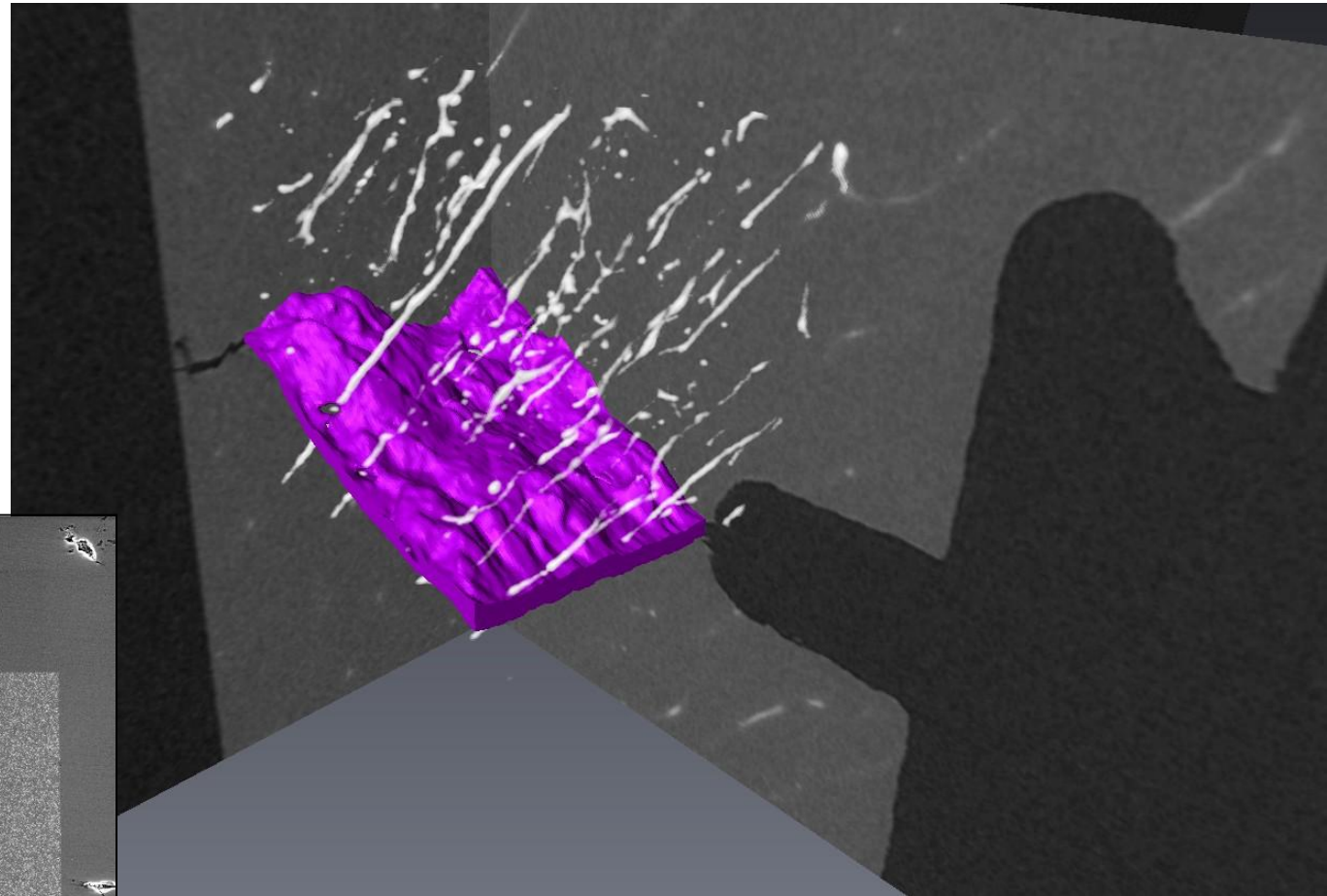


In-situ ESEM Strain Accumulation Measurement *single crystal Al-2Cu*

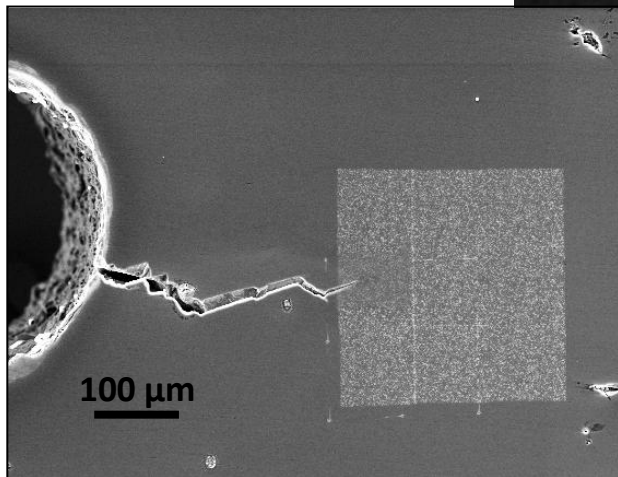


Al-Cu X-Ray CT Scan

Can we control propagation path by designing precipitate structures?



Single crystal Al-2Cu



Summary for Al-Cu



- Fabrication of single/bi-crystals and large-grain polycrystalline specimens of Al-Cu alloys provides a less complex material of study.
- High-resolution image correlation combined with EBSD can provide more detailed information on validity of crystal plasticity models.
- Calibration of critical cracking criteria at this scale can be obtained by correlating computed and measured results.
- Full-field strain data should eventually provide a means to determine the variation in material parameters across a microstructure.

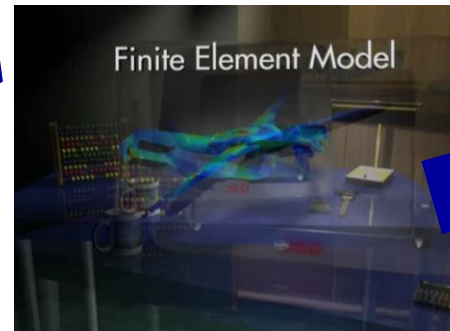
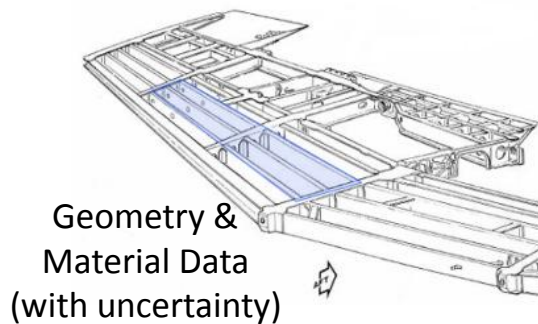
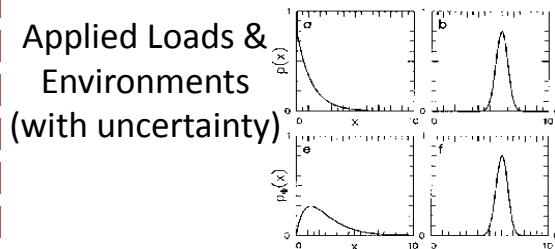
Outline



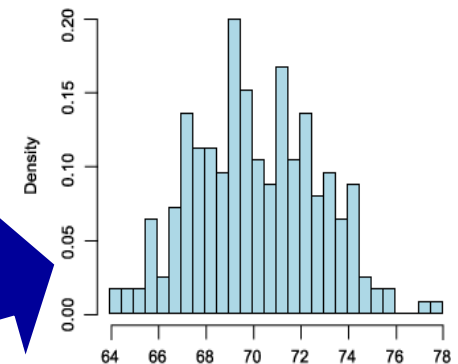
- Brief branch portfolio (collaborations)
 - Ni superalloy
 - Crack locating
- Materials Genome Initiative (MGI)
 - Fabrication and testing of various Al-Cu alloys
- **Airframe Digital Twin (ADT)**
 - Embedded shape memory alloy particles as crack detection sensors

Airframe Digital Twin Concept

Model the **as-built** vehicle component(s) and **as-experienced** loads and environments throughout a vehicle's service life



Physics-based Multi-scale,
Multi-Discipline Models

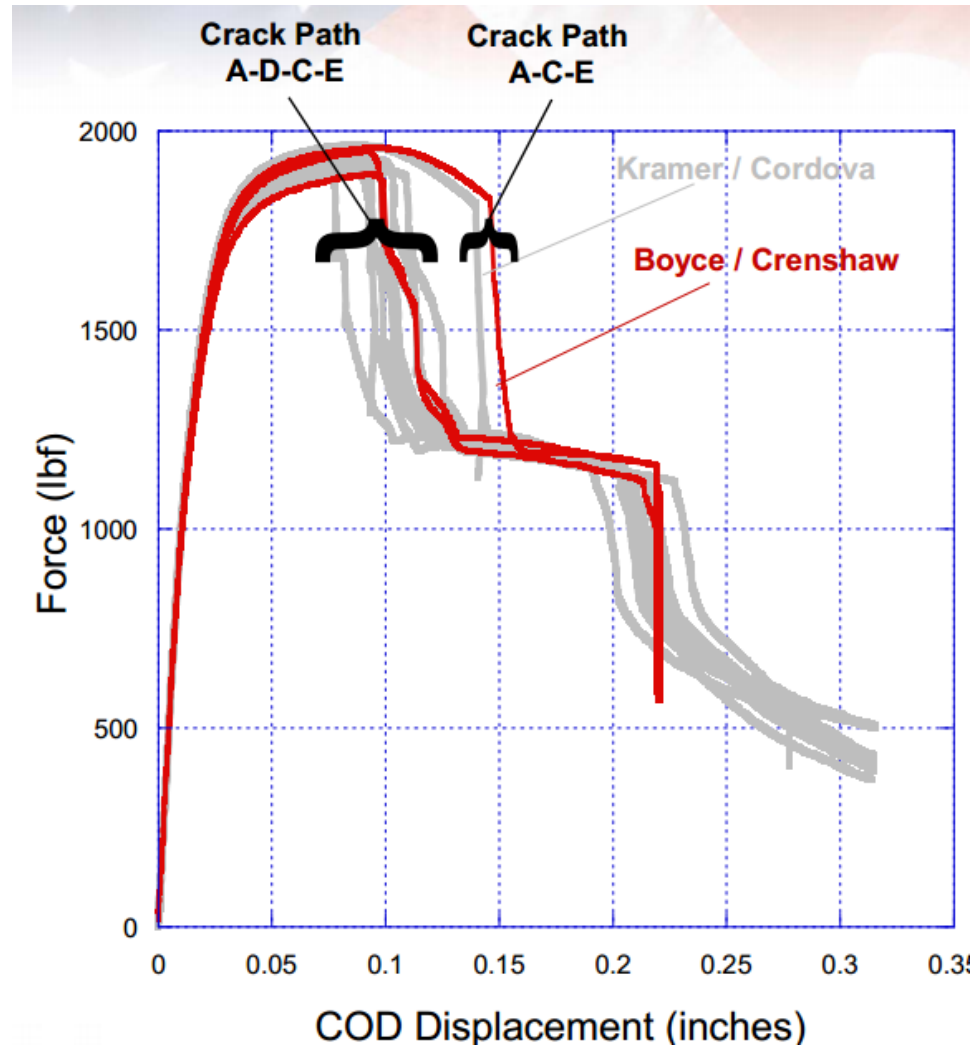
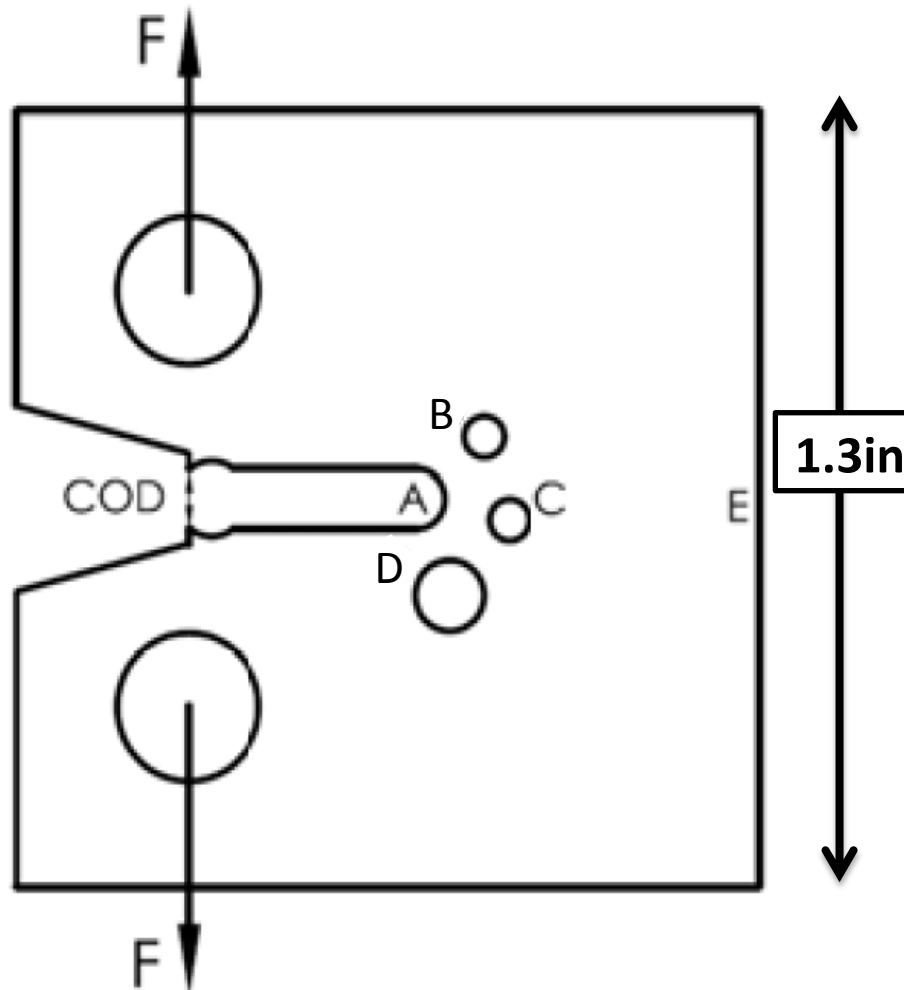


Range of Structural
Response & Reliability
(Probabilistic)

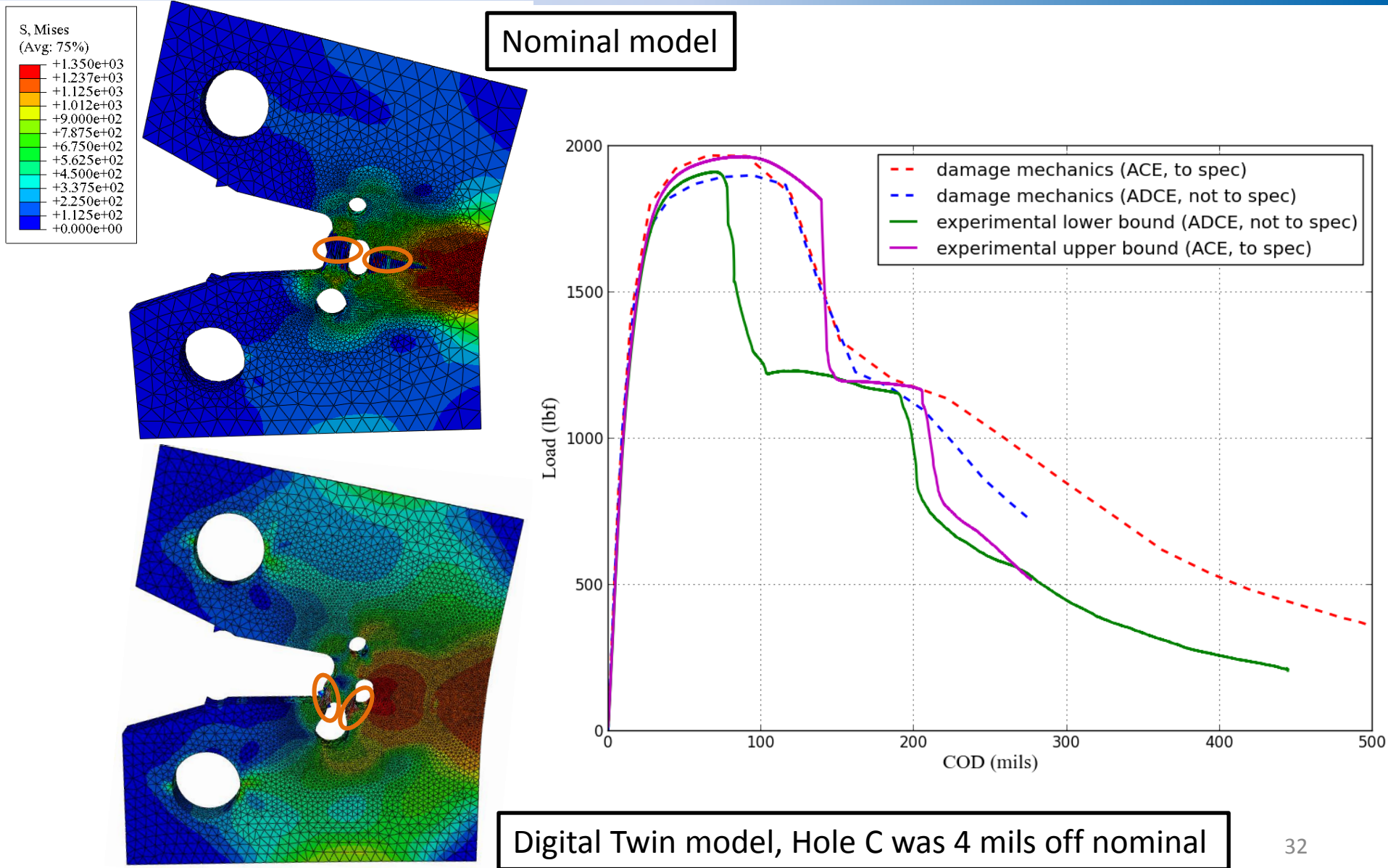
Airframe Digital Twin Usage Case



The National Fracture Challenge Problem - SANDIA NL



Airframe Digital Twin Usage Case

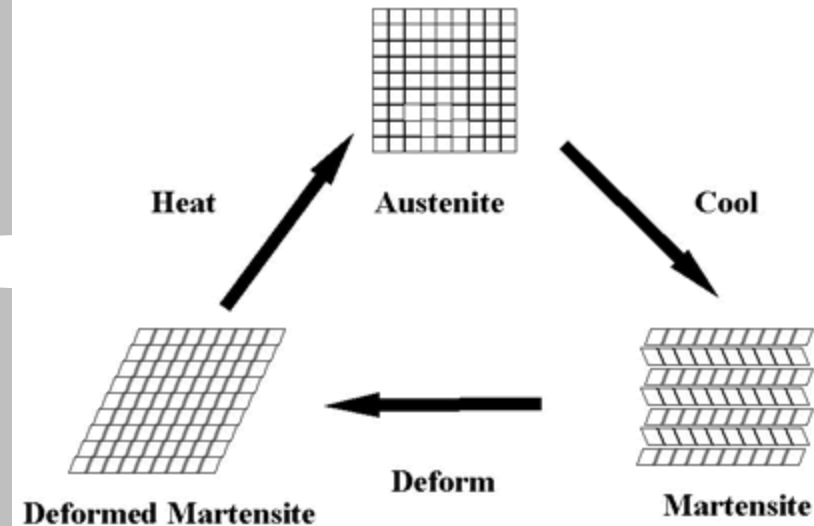
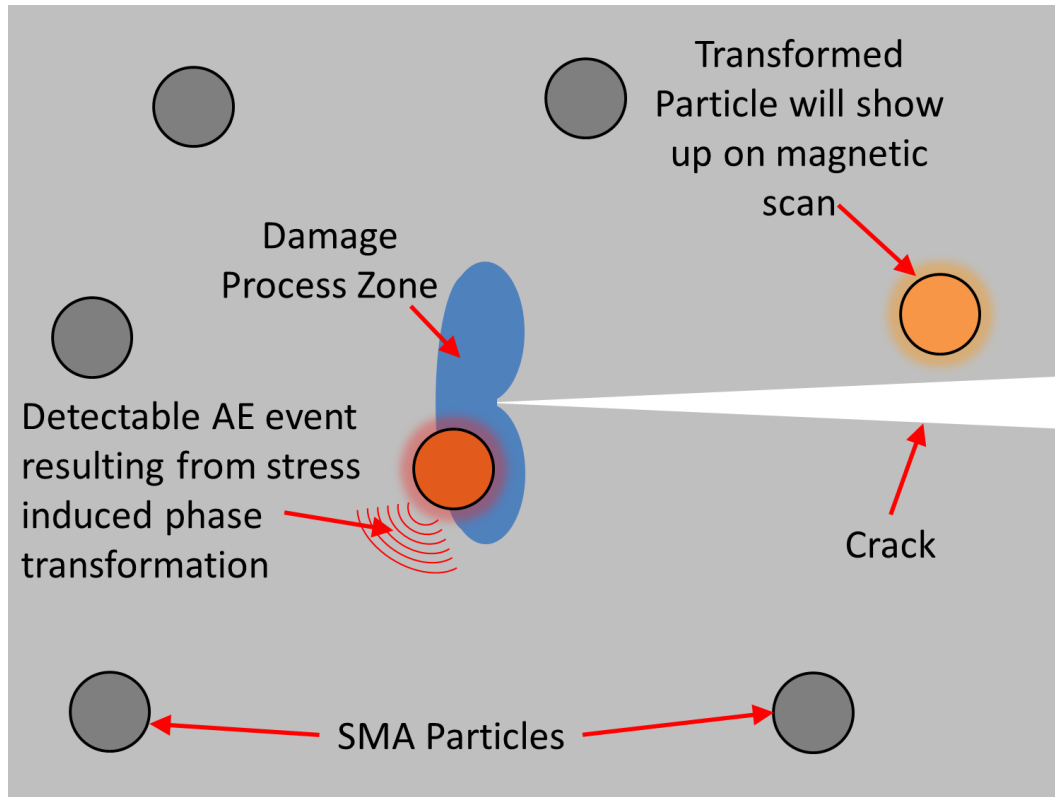


Outline



- Sensory particle behavior
 - Processing temperature vs. Transformation strain
- Measuring full-field strain by image correlation
 - Bulk material calibration
 - Embedded particles
- X-Ray CT for 3D digital twin models

Sensory Particles



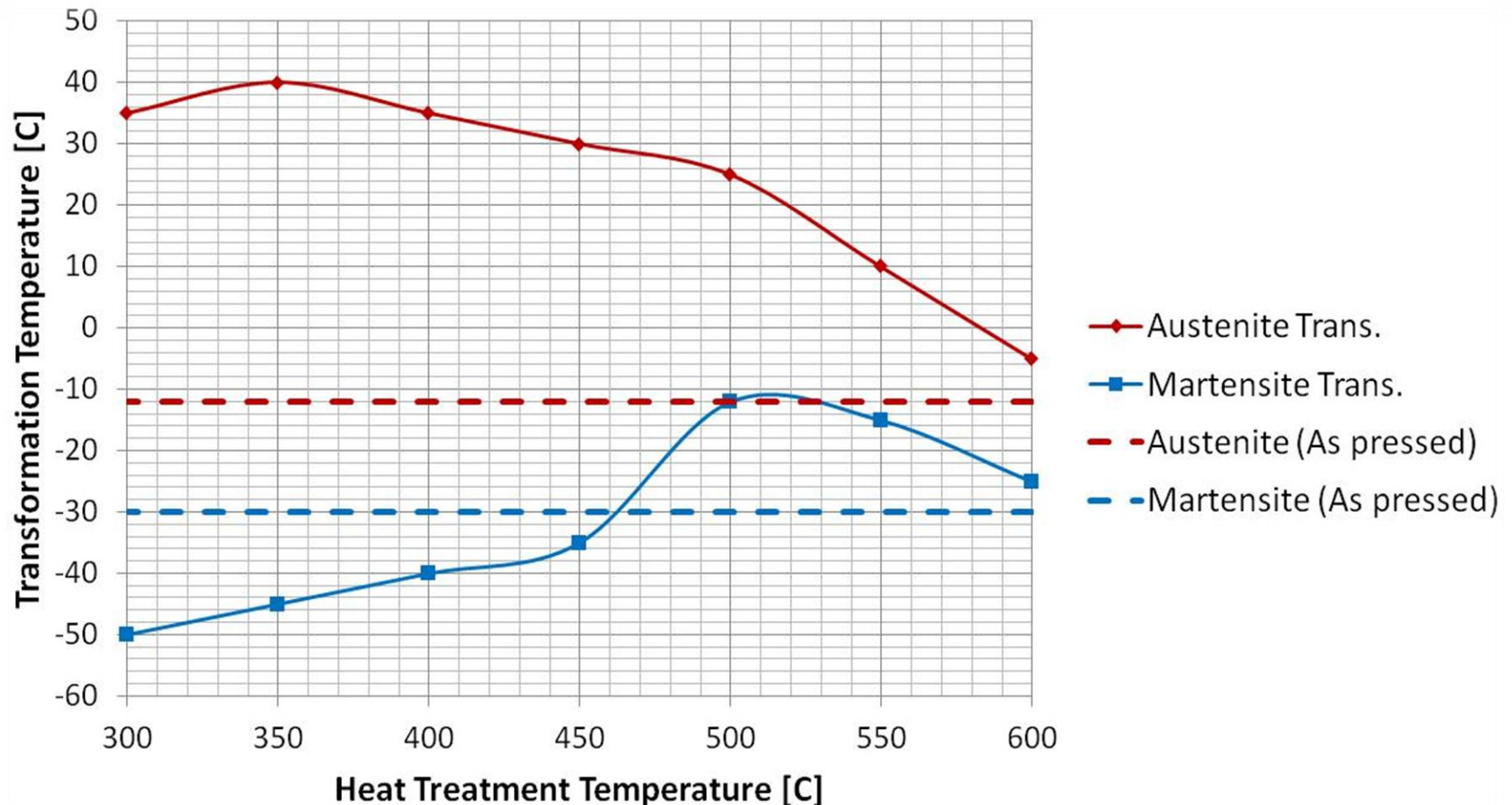
2 questions to answer:

- 1) At what strain (range) should they transform?
- 2) Is the transformation strain controllable?

Sensory Particles: Transformation Temperature



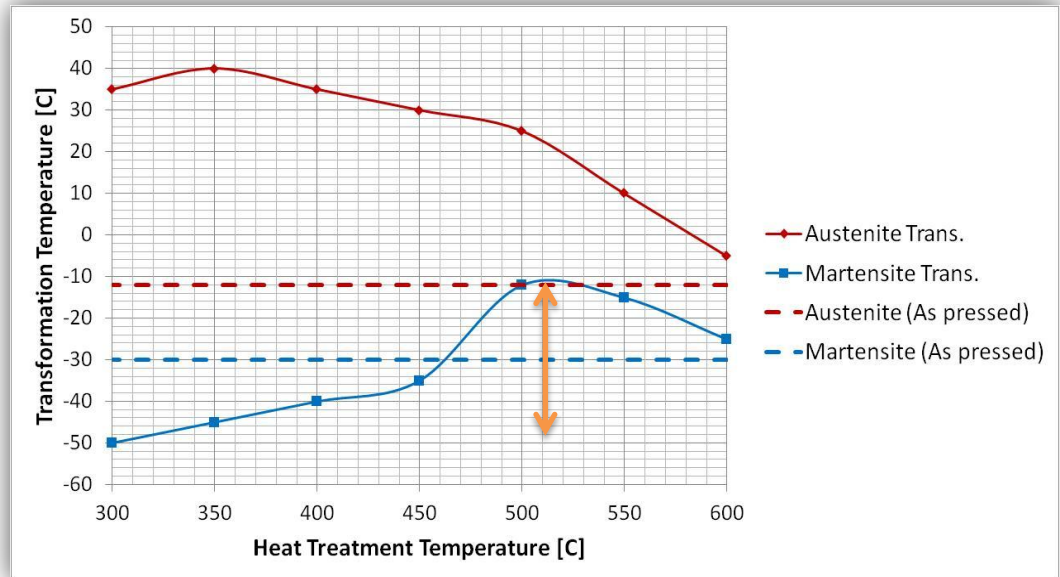
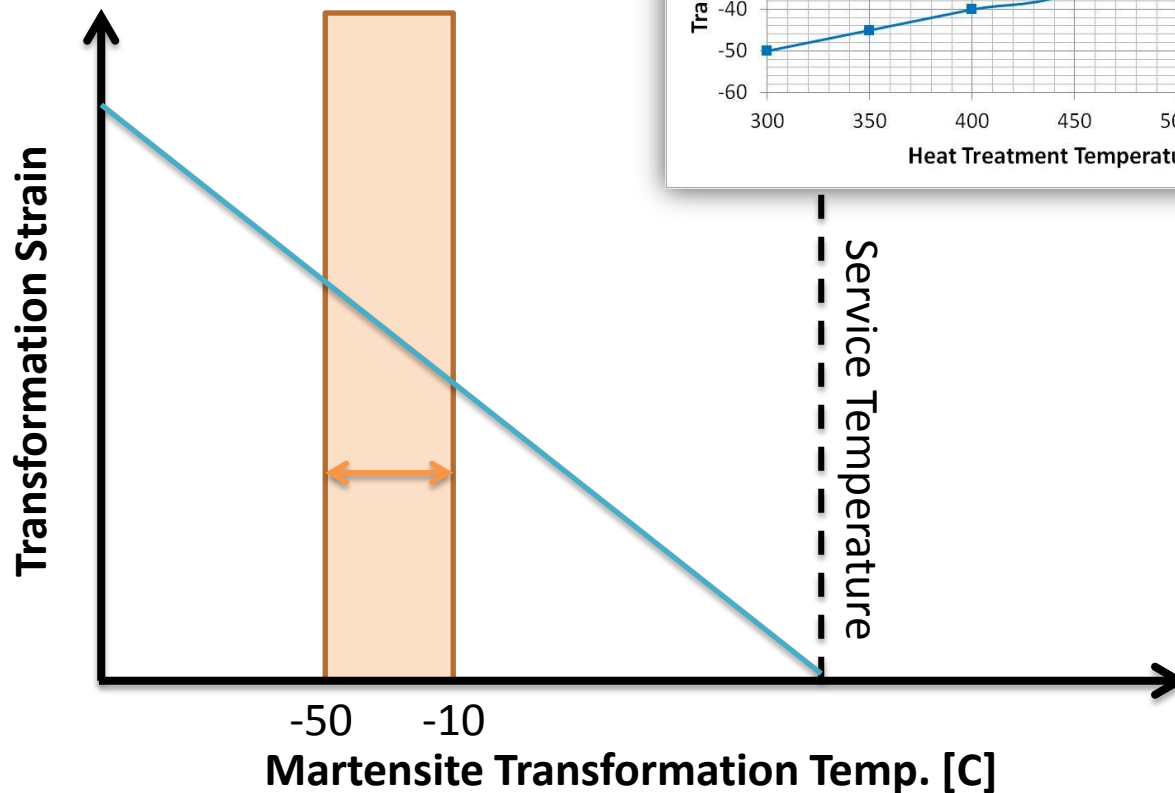
- Vacuum hot-pressed NiTi (50.9% Ni at.%; 56.0 Ni wt.%) @ 1000 C
- Relatively quick measurements using differential scanning calorimetry (DSC)



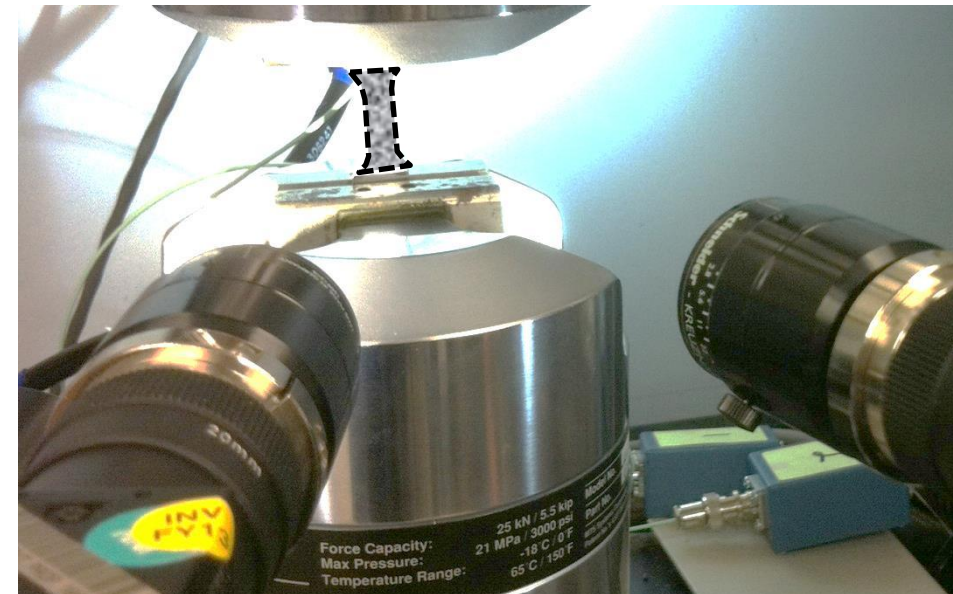
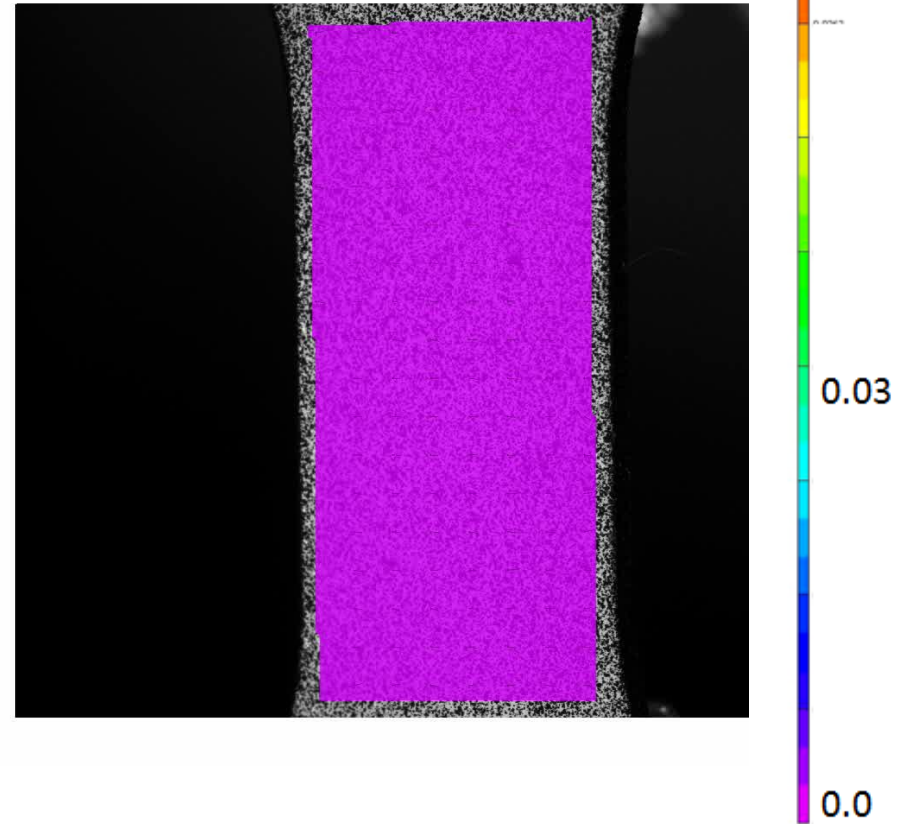
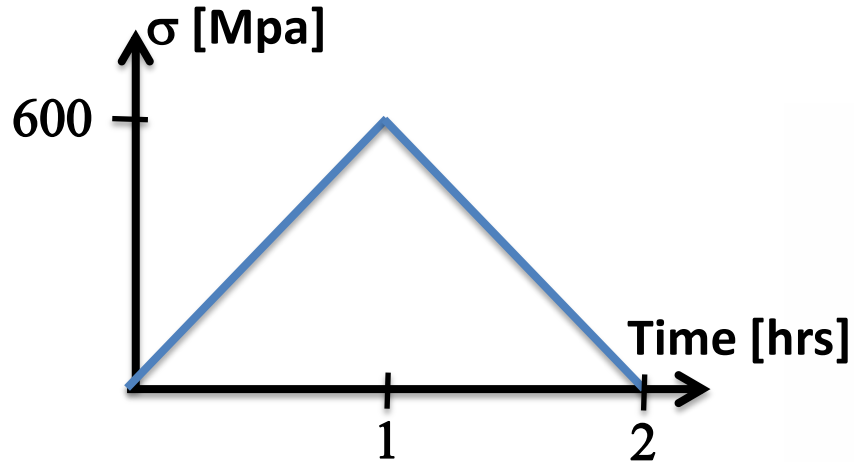
Sensory Particles: Transformation Strain



Linking transformation temperature to strain



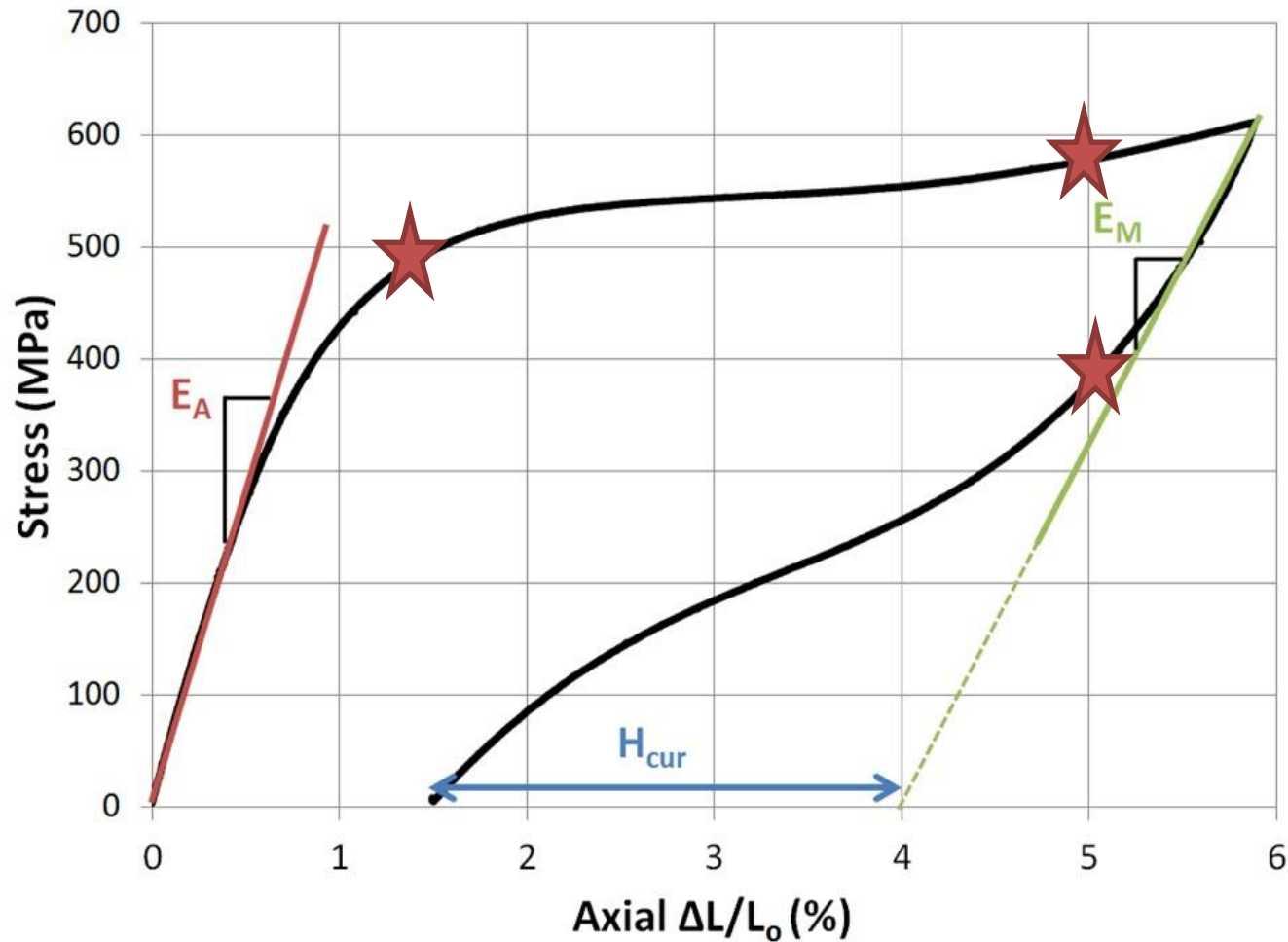
Bulk Material: Image Correlation



Bulk Material: Measured Behavior

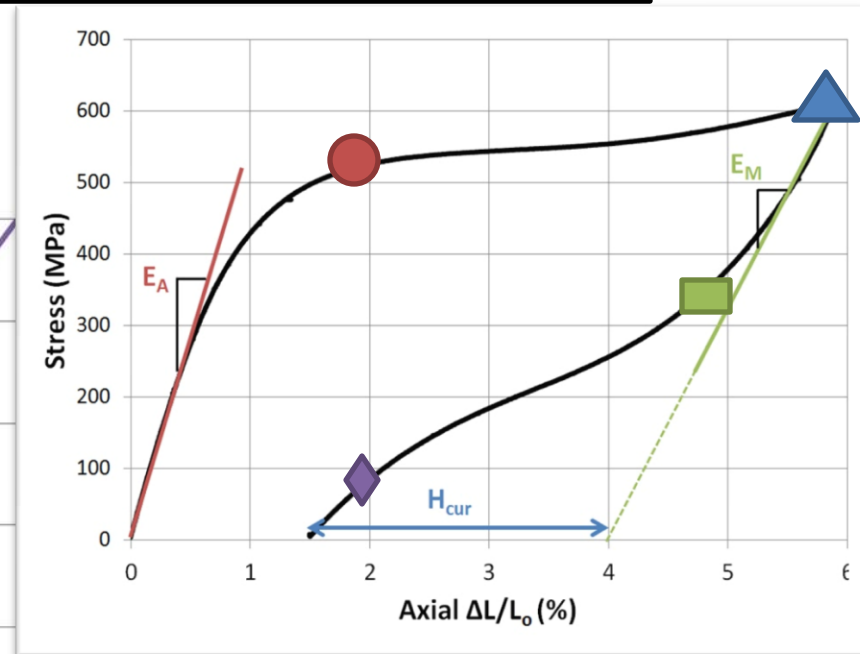
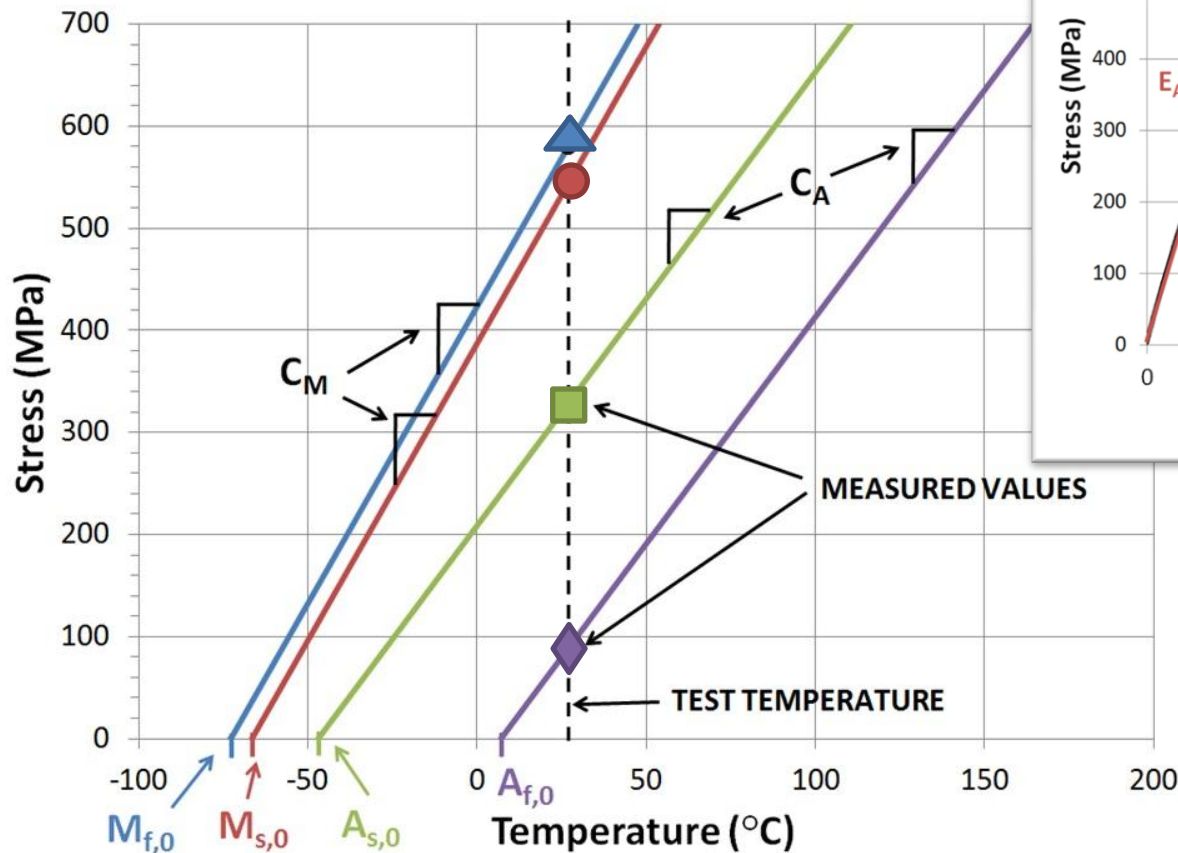


★ Indicates a burst of acoustic events

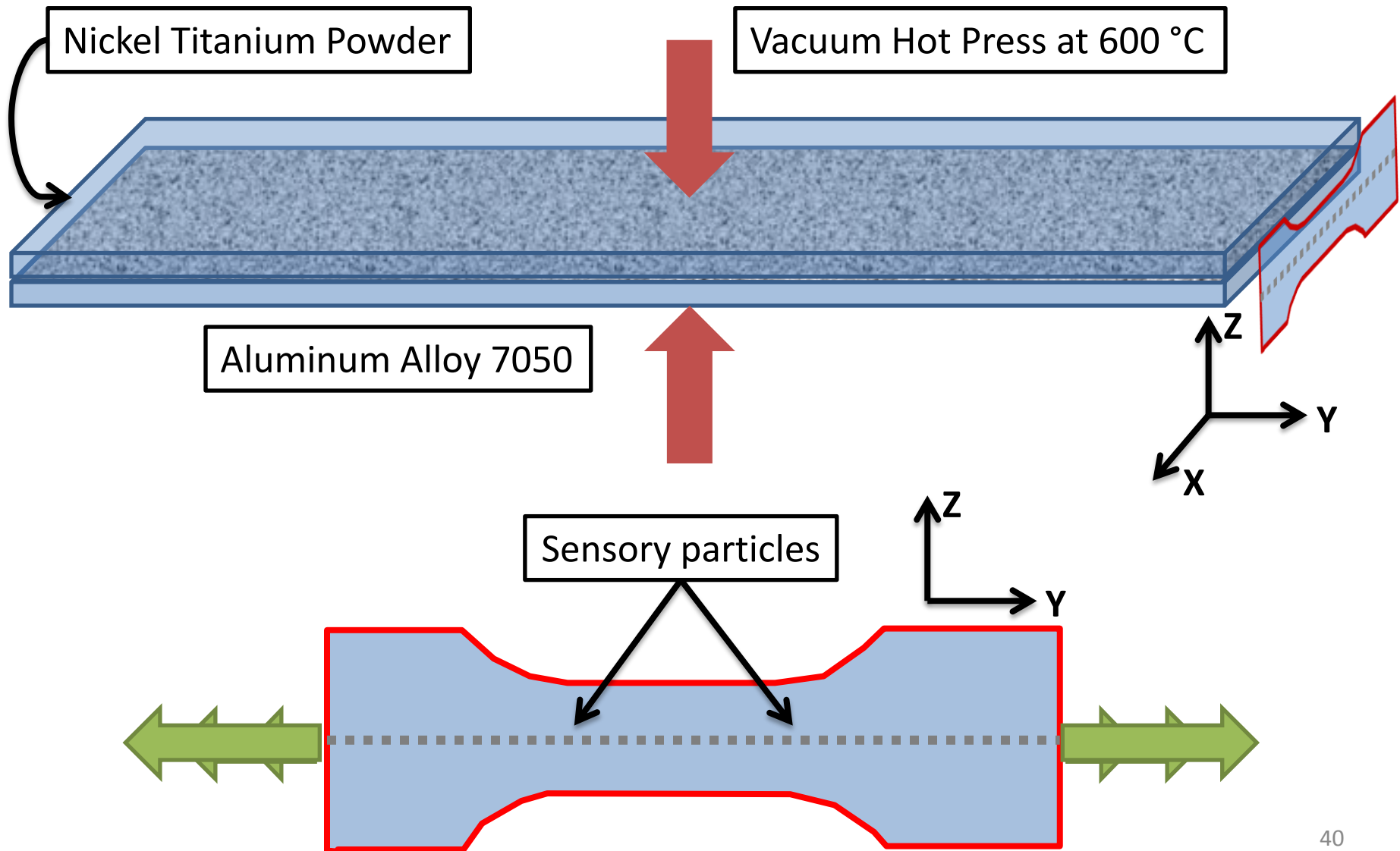


Bulk Material: Calibration

- Currently only studying behavior at room temperature
- Testing at various temperature still need for full calibration



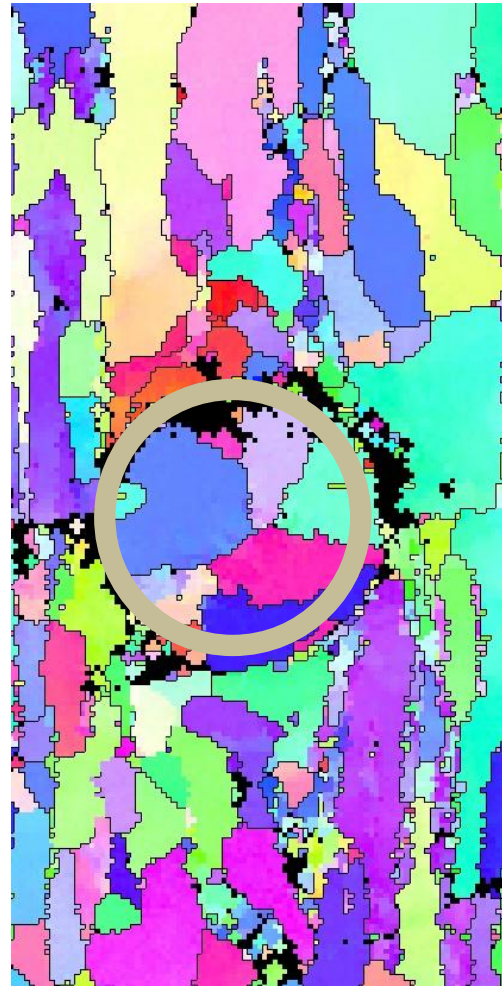
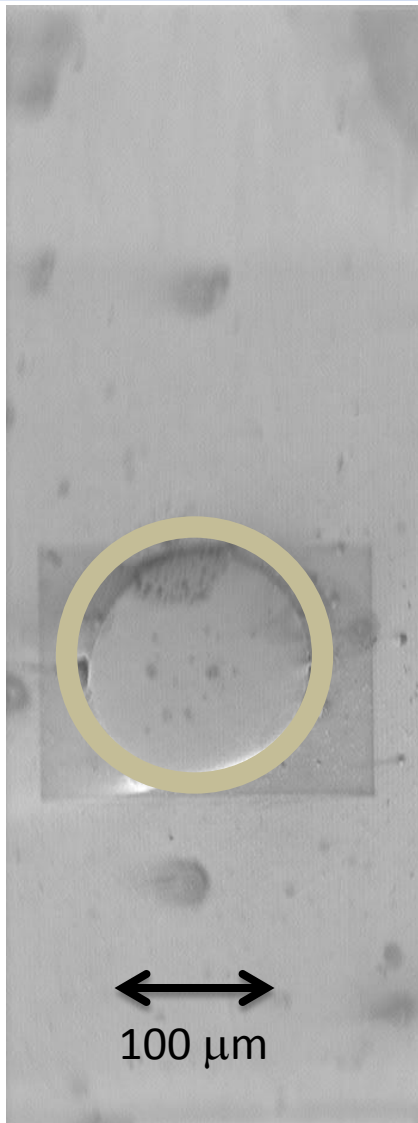
Sensory Particles: Specimen Fabrication



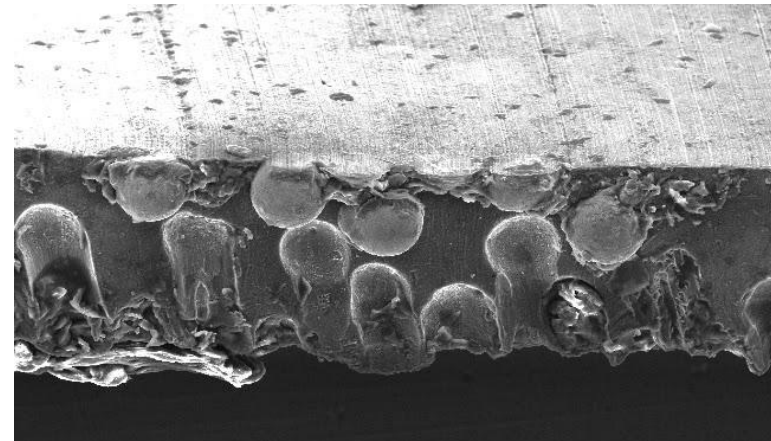
Sensory Particles: Microstructure Analysis



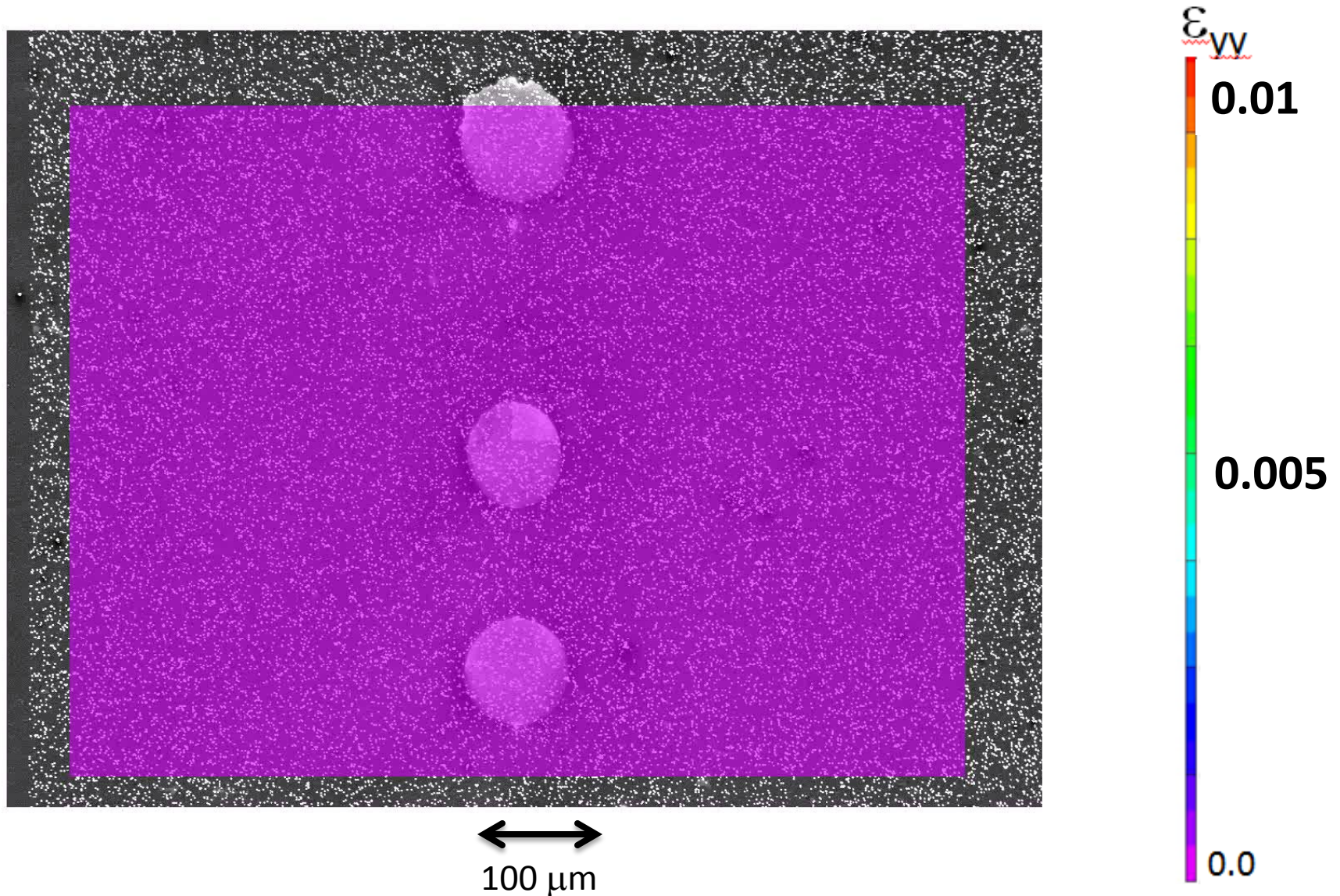
Electron Backscatter
Diffraction



Debonded particles

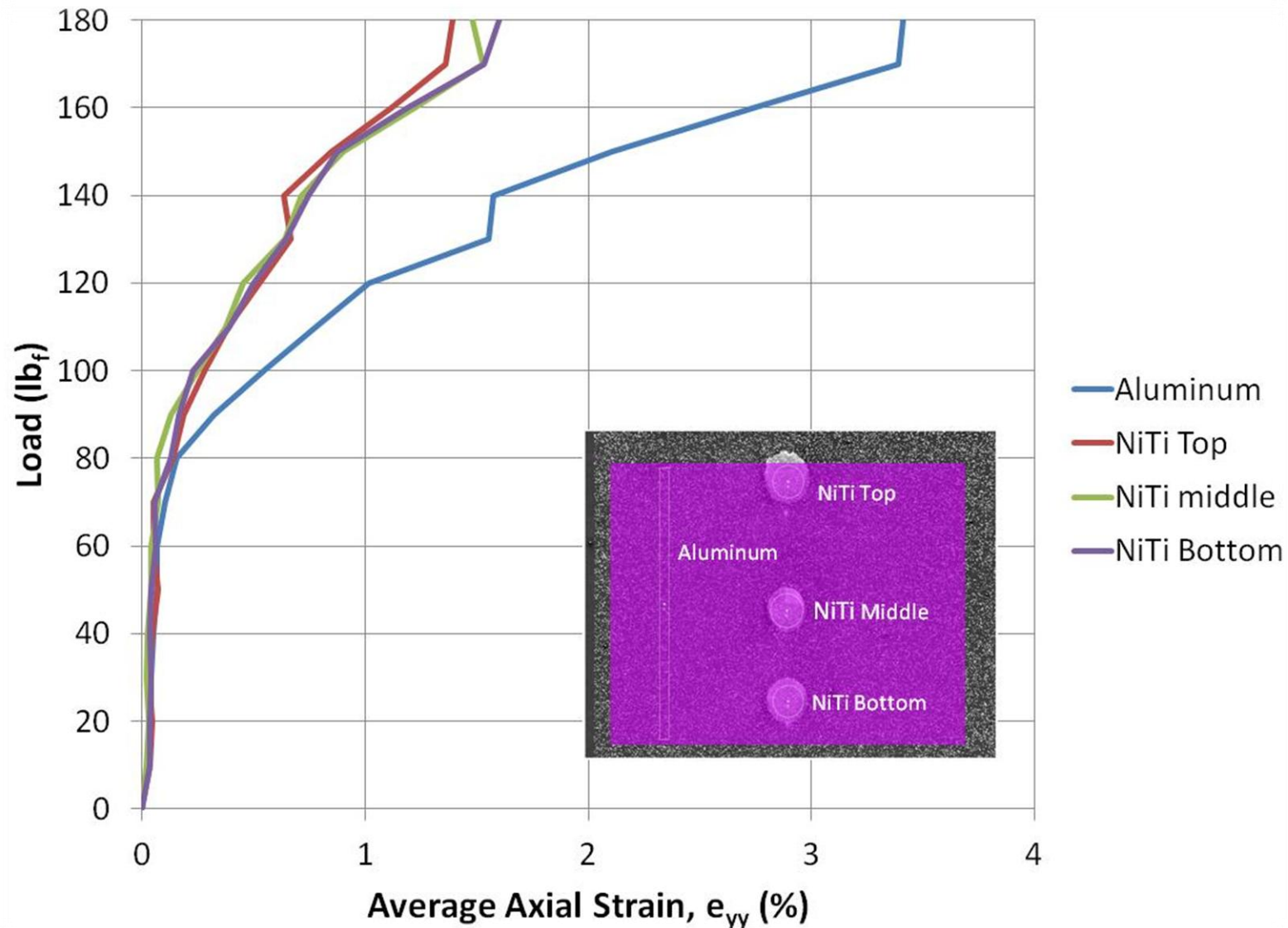


Sensory Particles: Image Correlation





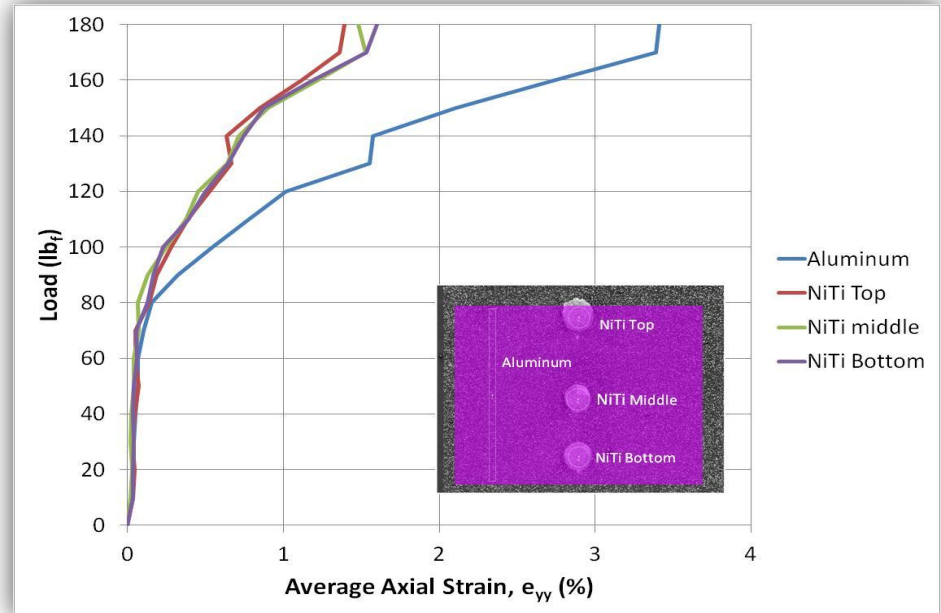
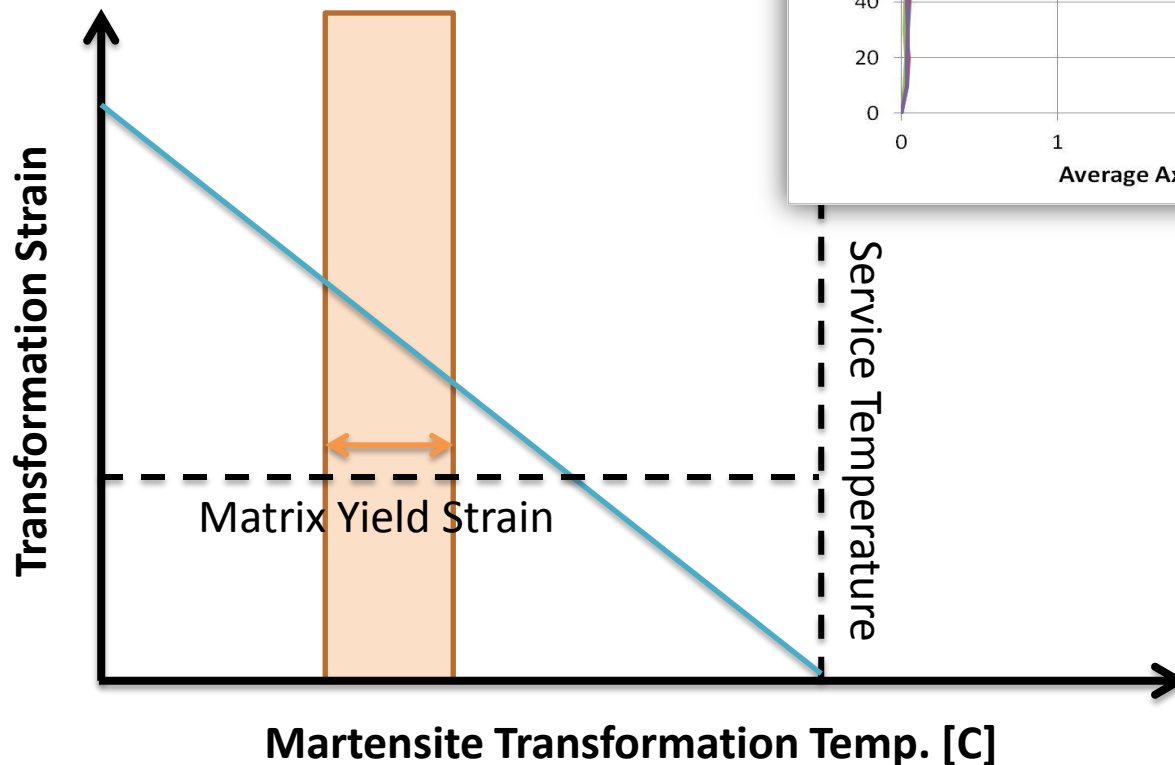
Sensory Particles: Measured Behavior



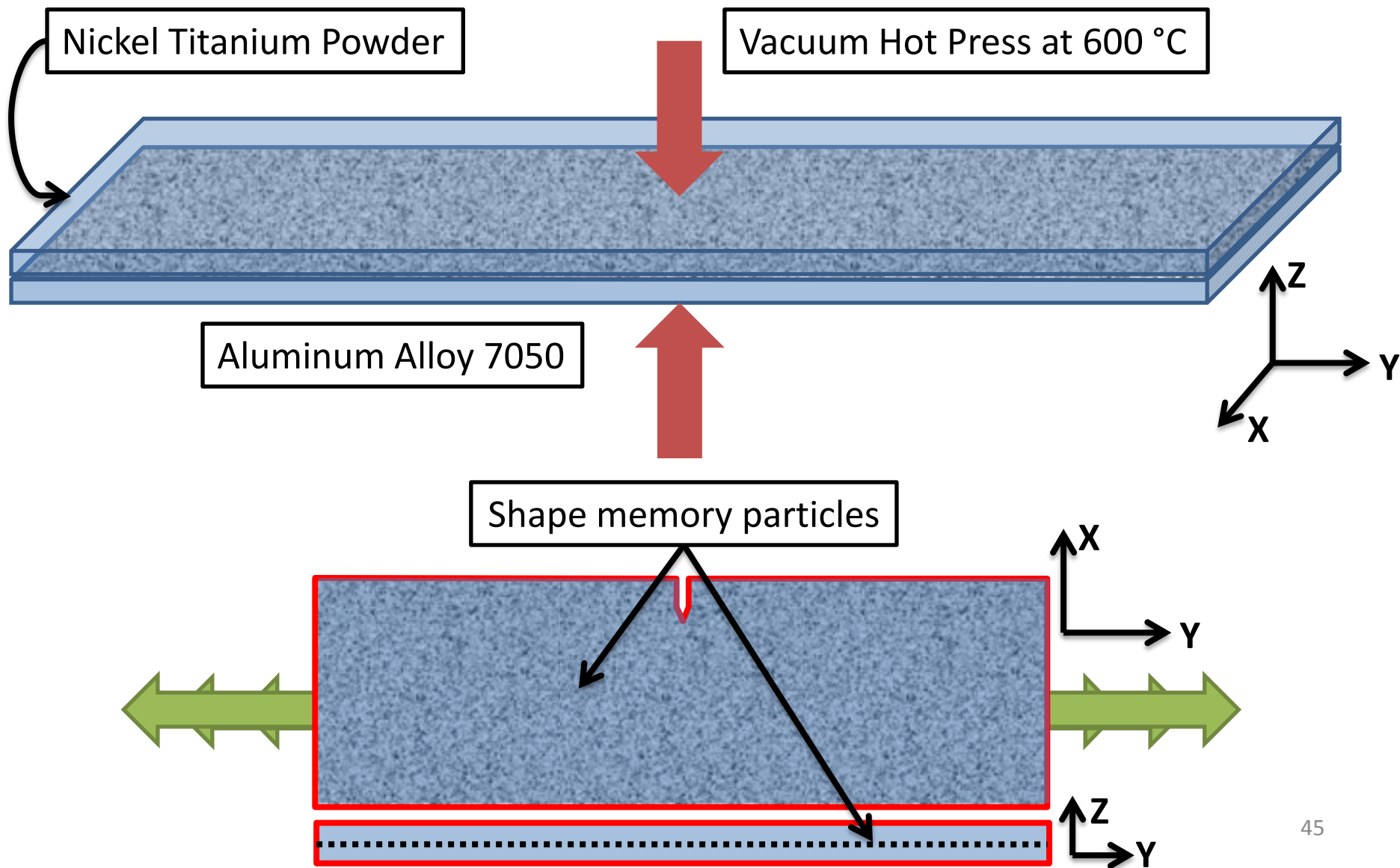
Sensory Particles: Transformation Strain



Targeting a transformation strain



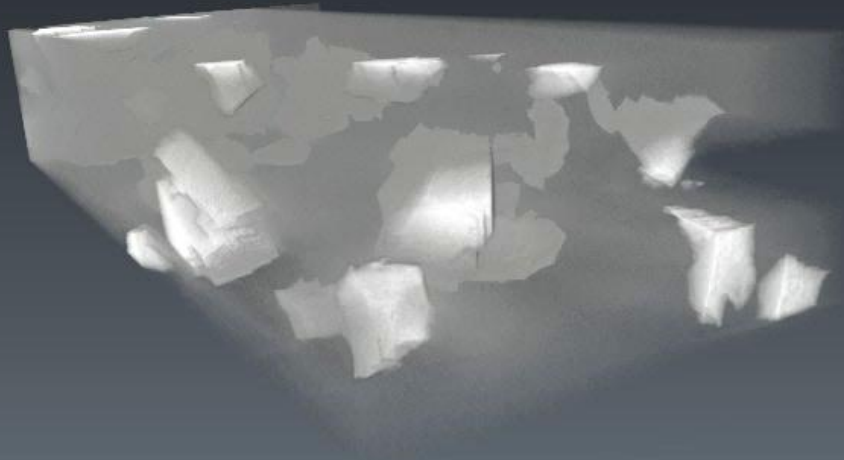
Sensory Particles: Specimen Fabrication



Sensory Particles: Generating the Digital Twin



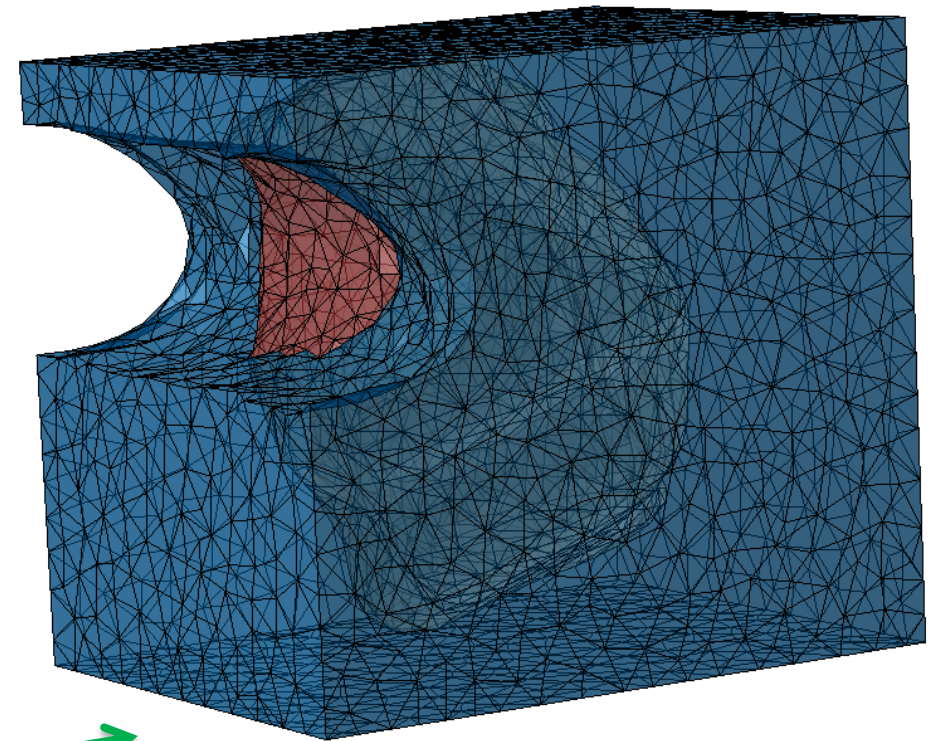
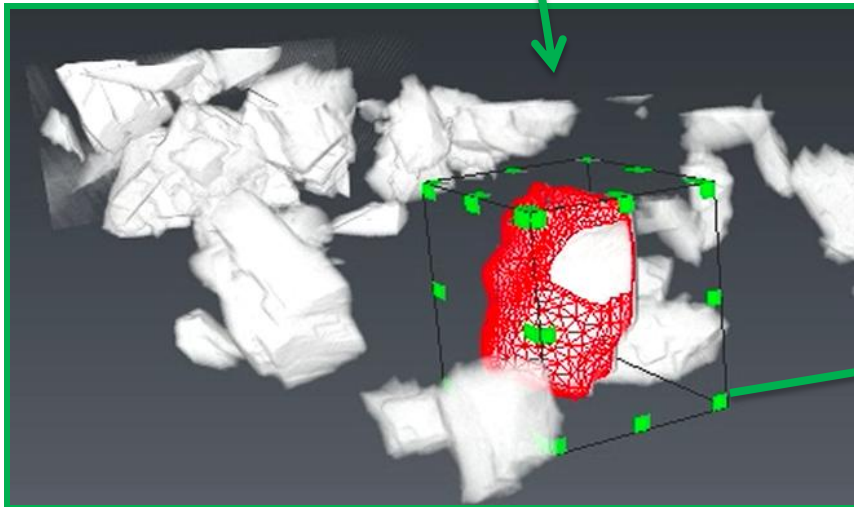
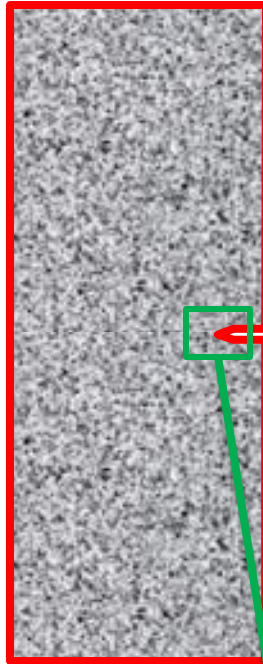
...using X-ray Computed Tomography



Sensory Particles: Generating the Digital Twin



Finite element mesh on an
embedded particle of interest



Summary of NiTi



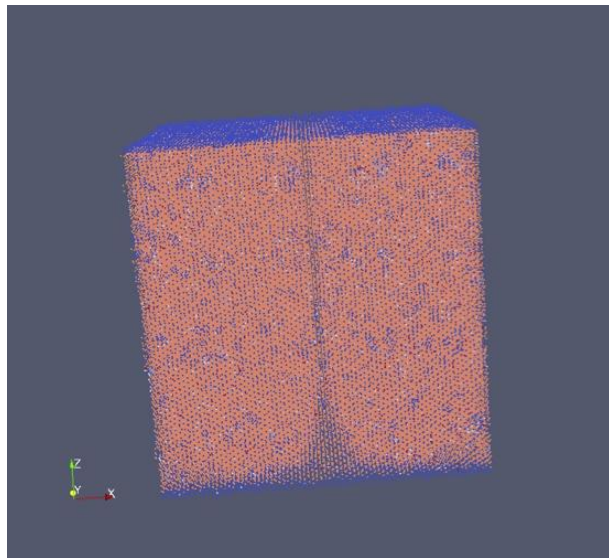
- Off-the-shelf NiTi powder provides a detectable acoustic emission upon transformation under load.
- Calibrated an ABAQUS UMAT for modeling the shape memory behavior.
- Still testing various heat treatments to determine the correlation between transformation strain and fabrication parameters.
- When embedded in an Al alloy, the 3D geometry can be measured precisely using Xray CT scans.
- The Xray CT scans can be used directly to generate the digital twin model of each specimen.

Molecular Dynamics (MD) Simulations

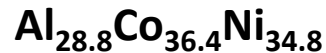


Starting System: B2-NiAl Cube of size 16.3 nm with periodic boundary conditions

Cooling/Heating the system: to study dynamically the martensitic phase transformation from Austenite to Martensite in CoNiAl ($T = 600 \rightarrow 200 \rightarrow 600$ K)



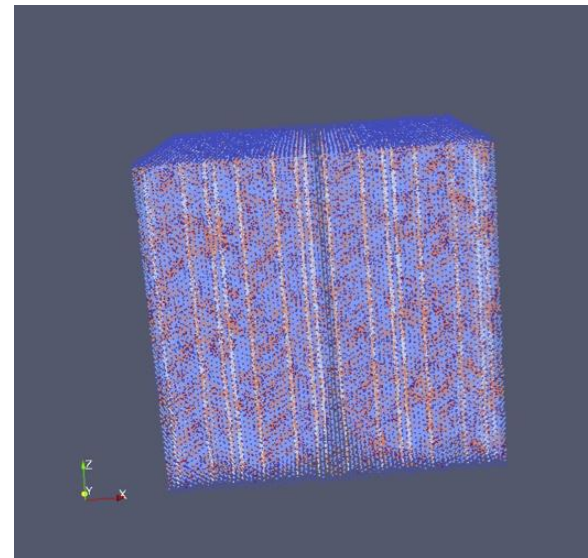
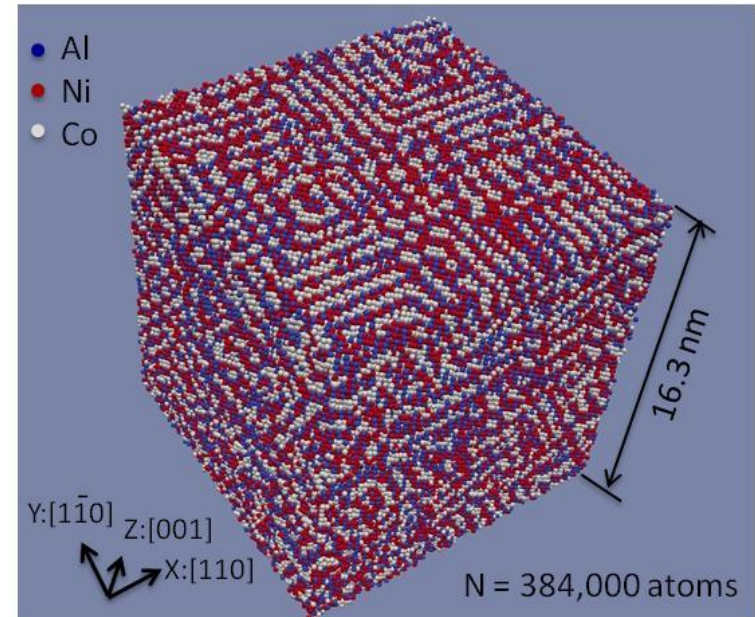
B2 – austenite



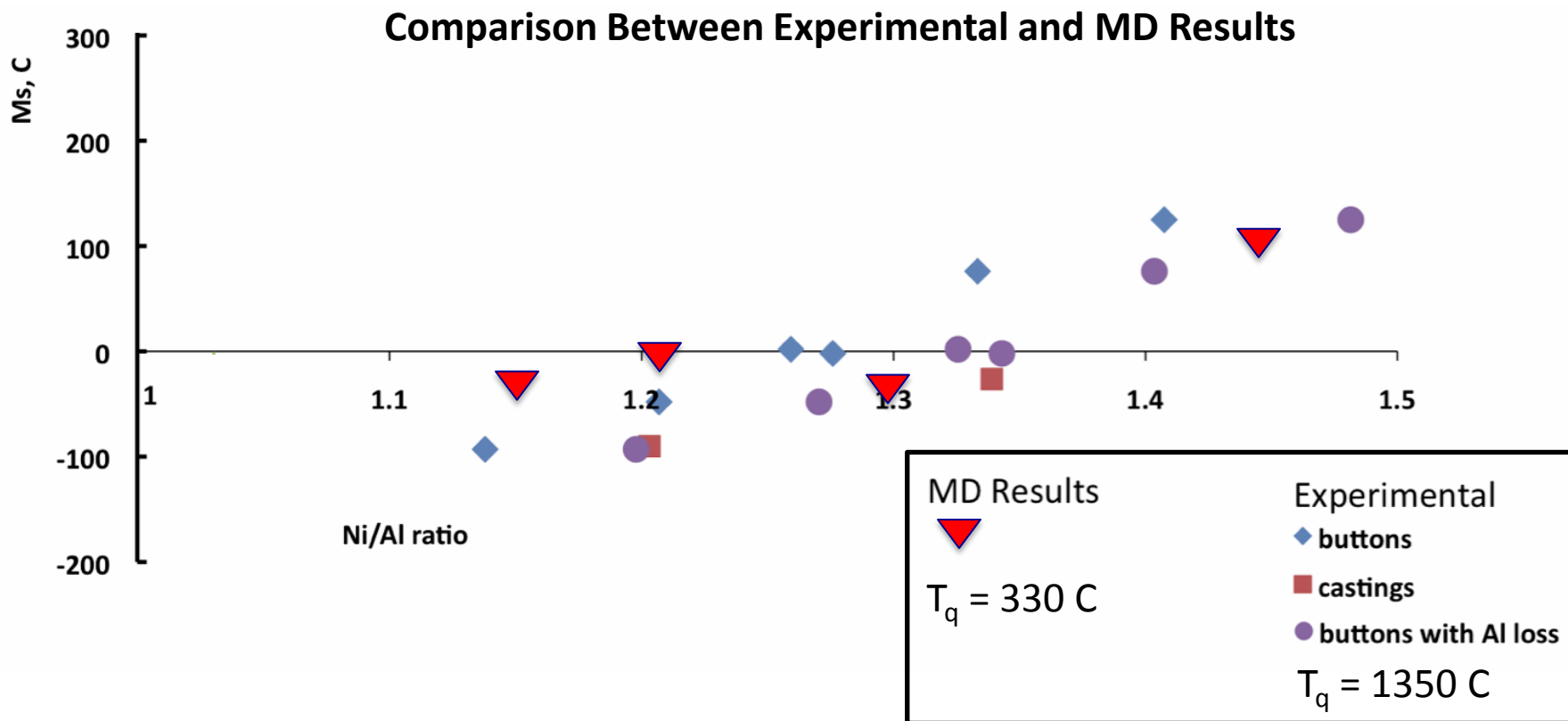
Common Neighbor Analyses identified atoms:

- bcc (B2)
- fcc (L1₀)
- hcp (twin)

L1₀ – twinned martensite



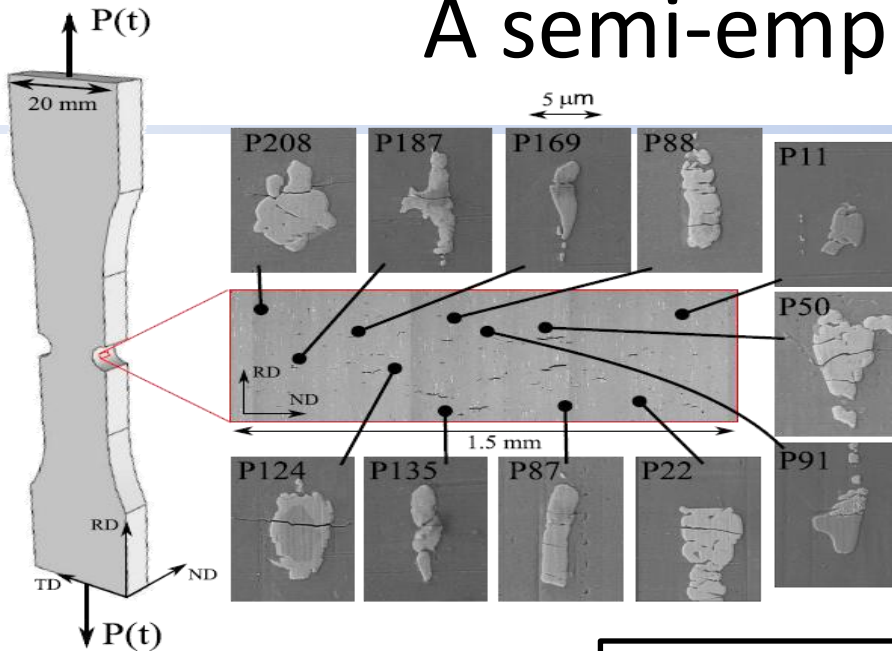
Downselect Chemistry from MD



MD simulations reproduce well the martensite transition for a range of compositions, but at a lower quench temperature!

Issue with the empirical potential or quenching rate (MD: 10^{12} K/s vs Exp: 10^3 K/s)?

A semi-empirical approach



Simulation of several microstructures led to a model that describes observed variability

