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Coupling damage-sensing particles and computational micromechanics to enable the digital twin concept

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What do we do?

Address certification and reliability issues that are limiting aerospace technologies

Past research supporting damage tolerance has relied on:
- Extensive testing under assumed representative service conditions
- Ability to find and repair damage before it becomes critical

Future missions are characterized by:
- Loads and environments that are not repeatable in the lab
- Vehicles that are not accessible for manual repair

Requisite research to get us there:
- Develop physics models to reduce reliance on testing
- Close coupling of sensor network and high-fidelity computational models for prognosis
- Develop autonomous damage sensing and healing technologies

Increasing requirements for long-term durability/performance
Decreasing ability to inspect/repair
Increasing requirements for novel materials, autonomous maintenance

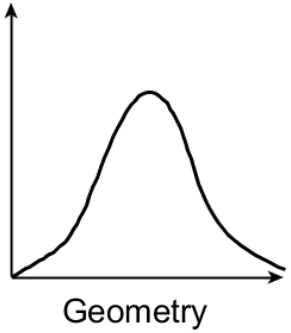
Outline

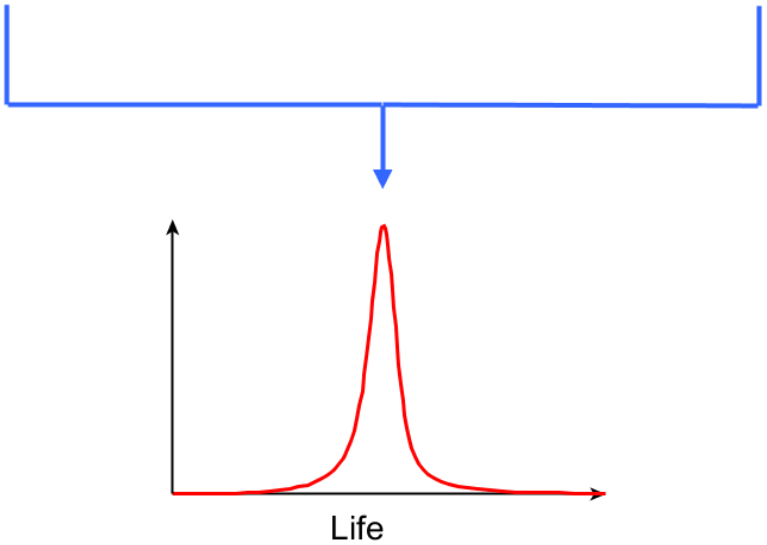
- Uncertainty, and what it means for design, certification, and maintenance standards
- Digital Twin
  - Concept
  - Geometric and Material Uncertainties
- Sensory Particles
- Encompassing Example
- Other Related and Requisite Technology
- Summary

How is it done now?

Gather Uncertainties

- leads to increased overall uncertainty in life predictions
- limits design space
- slows certification





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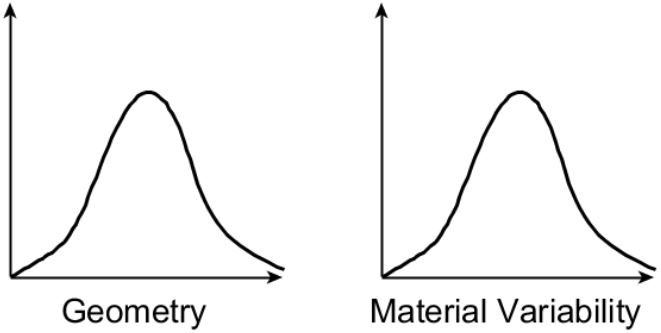

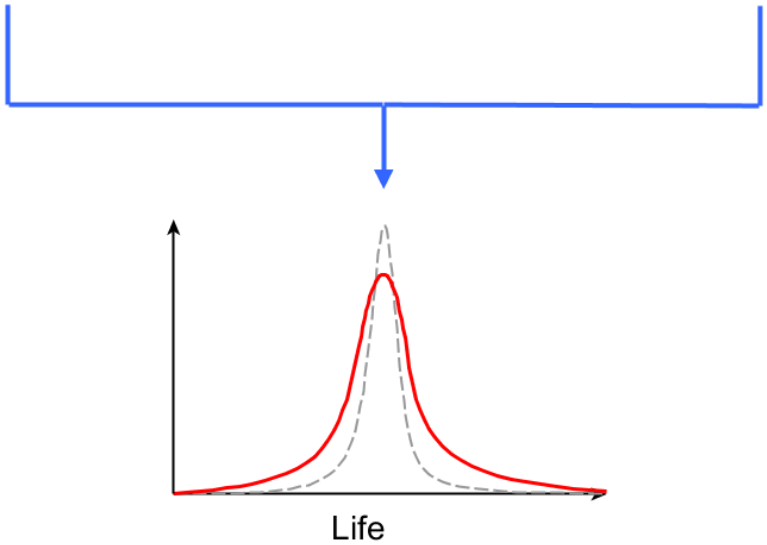

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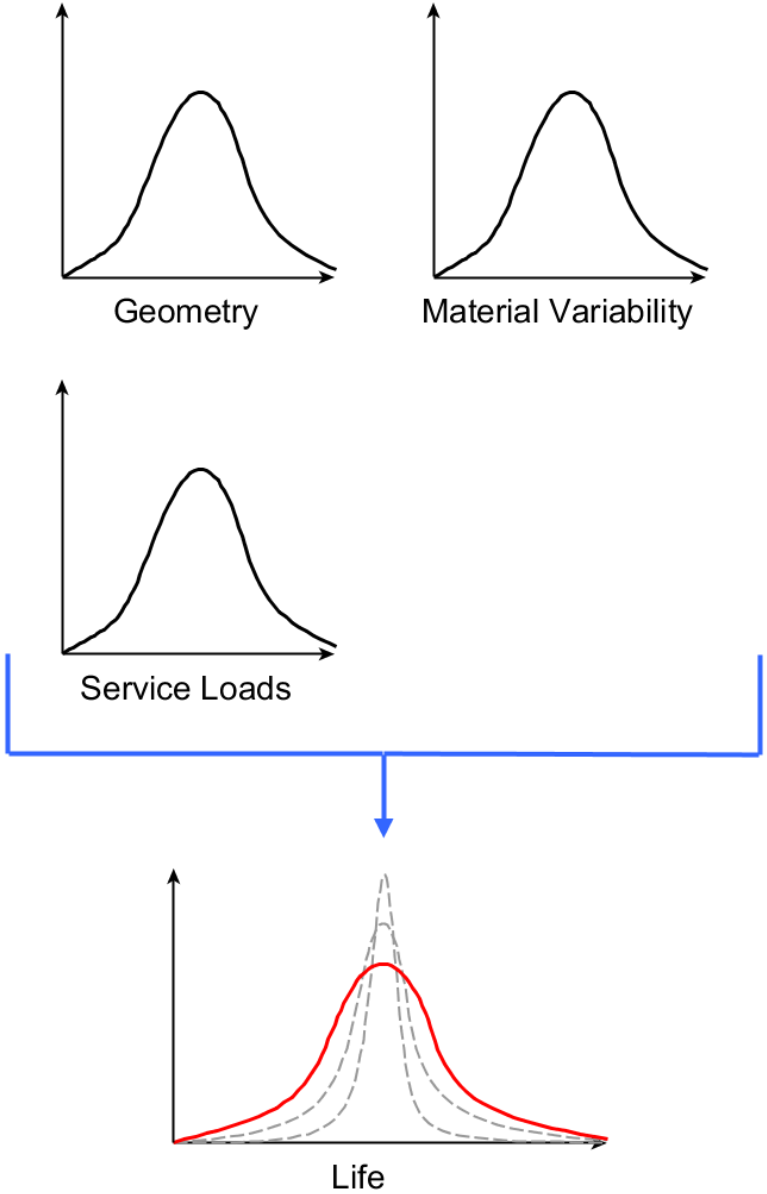

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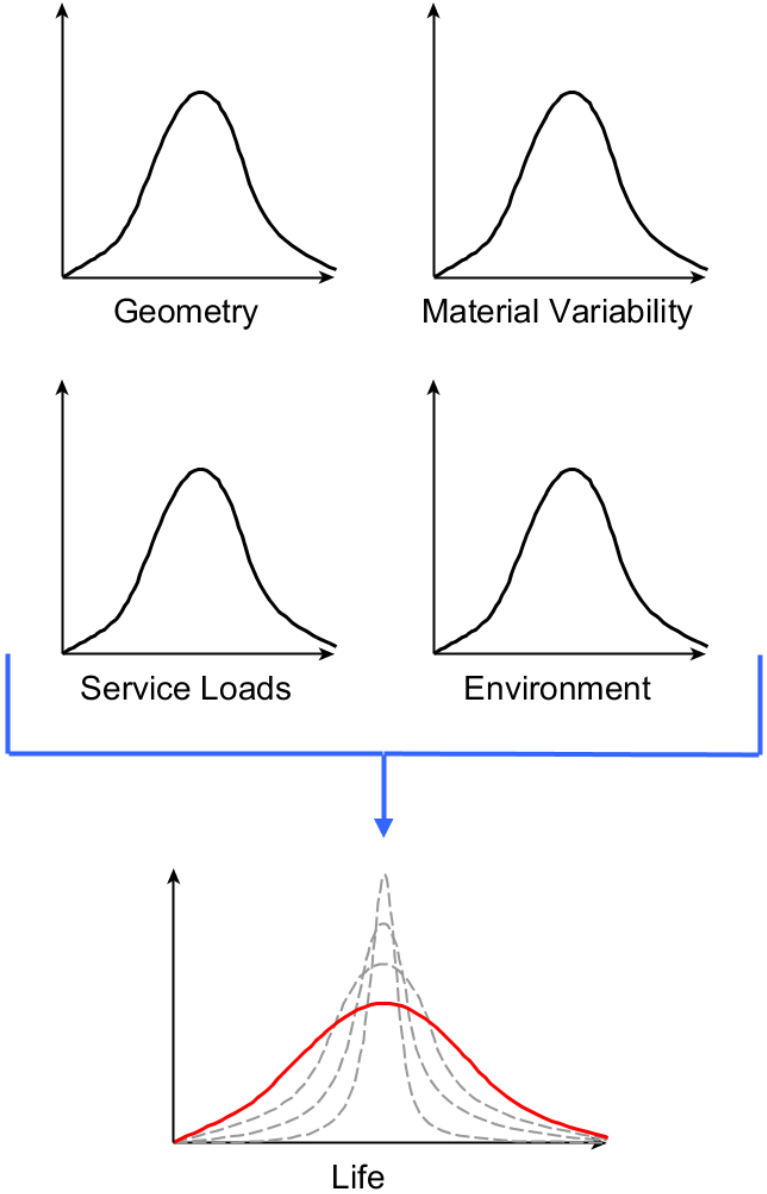


Objective

Big Question: How can we expand the design space and accelerate certification of n+3 structural configurations while assuring continued safety and reliability?

The Problem

- Overly-conservative design
  - Limits aircraft efficiency and performance
    - *e.g.* SUGAR II (Truss-braced wing)

The Problem

- Certification of new structural concepts and materials requires extensive testing programs
  - Cost and time prohibitive
    - *e.g.* Boeing 787

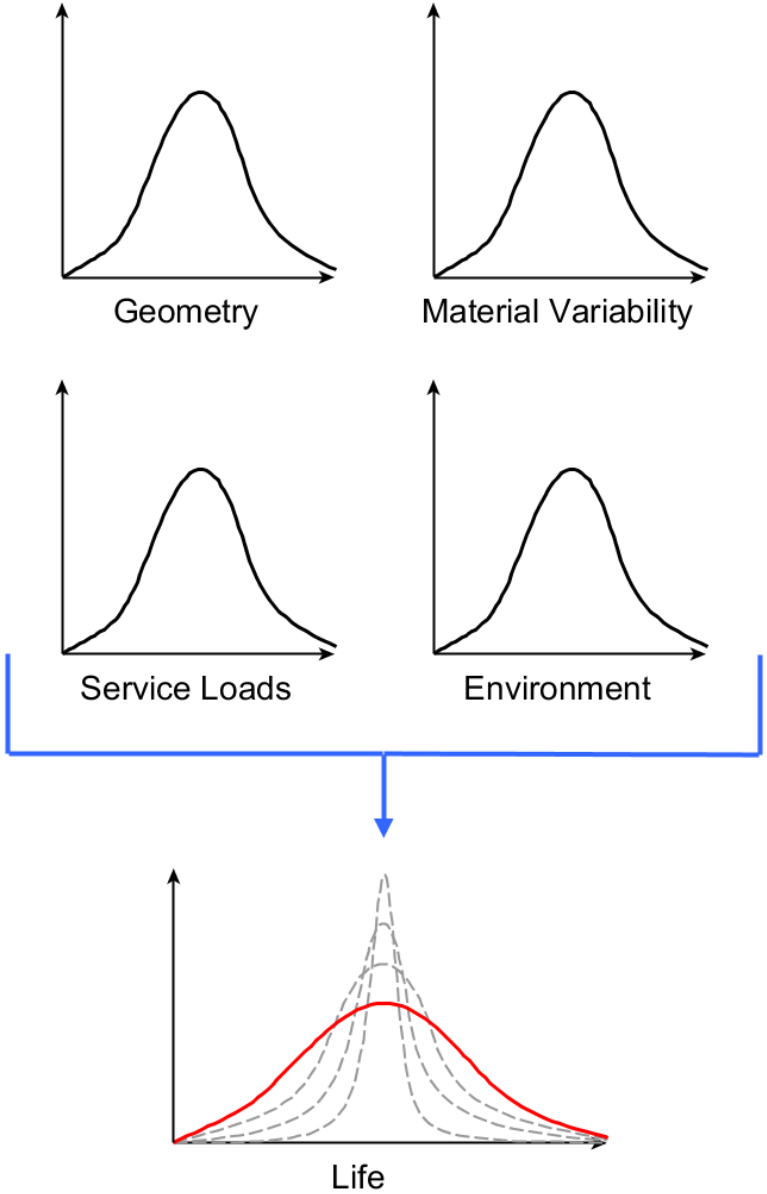
The Problem

- Maintenance is costly, time consuming and often unnecessary
  - *e.g.* USAF F-22

What can be done?

~~Gather~~ Reduce Uncertainties

- Epistemic – things we could measure (more accurately), but do not in practice
  - As-fabricated geometry
  - As-fabricated material data
- Aleatoric – statistical variation that can not be measured (more accurately)
  - Infer/update unforeseen phenomena, *e.g.* unknown damage modes.



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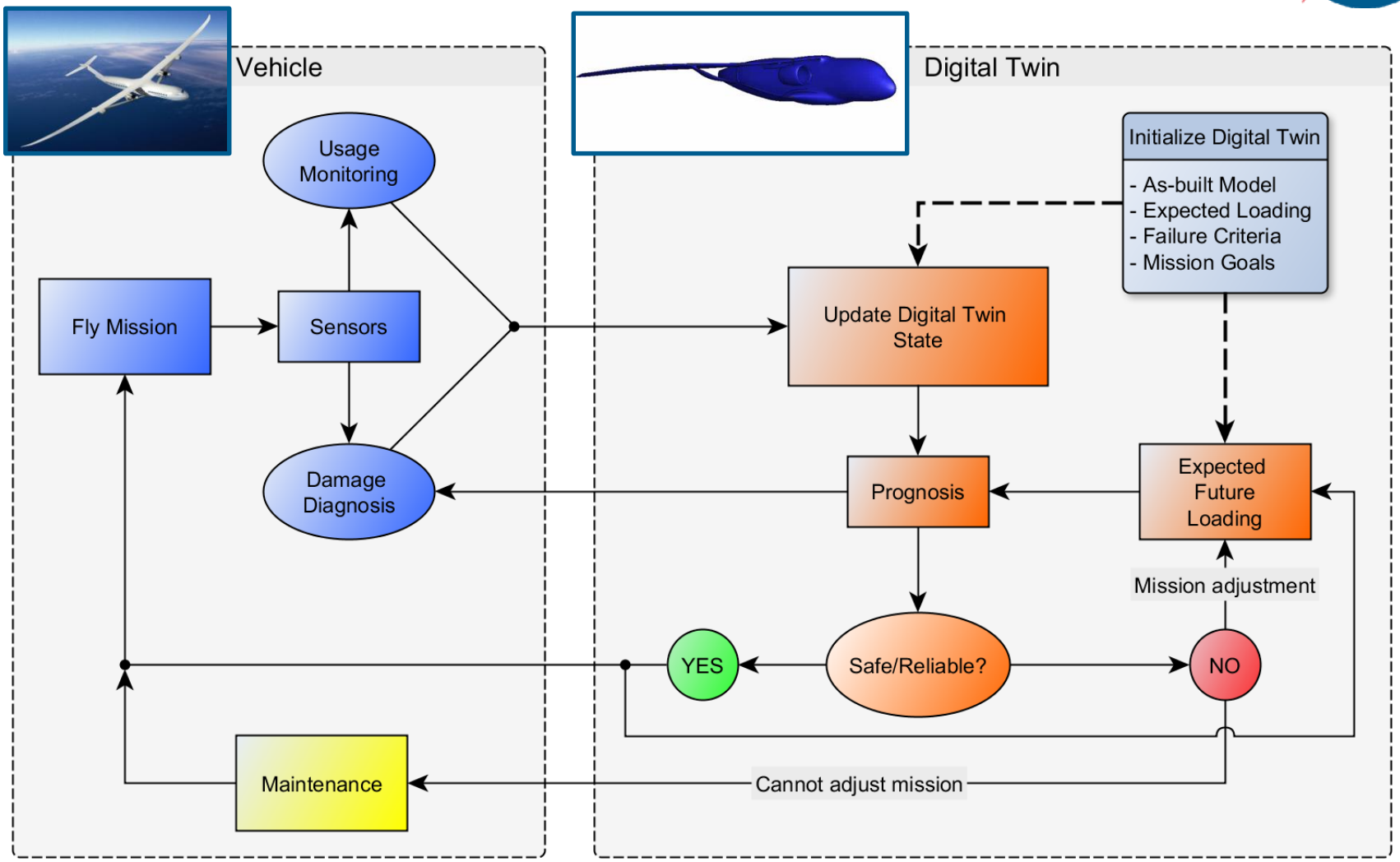
Digital Twin Concept

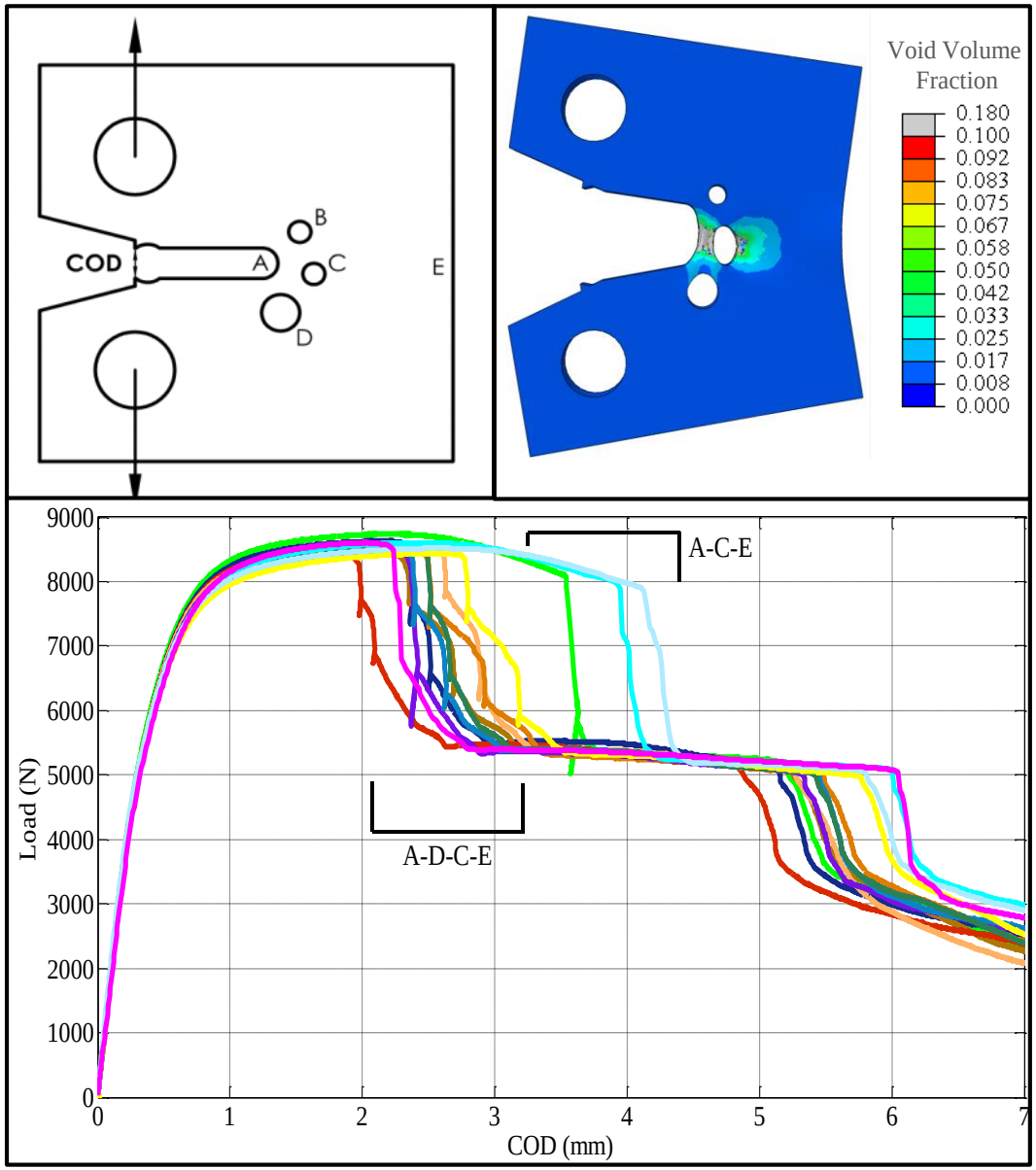


High-fidelity models informed by in-service usage monitoring

Reducing Epistemic Uncertainty: Geometry

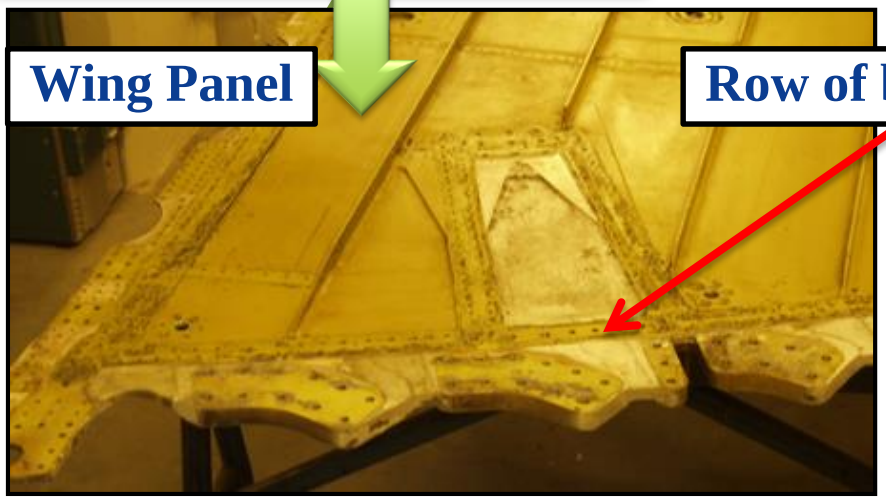
1st Sandia Fracture Challenge Problem

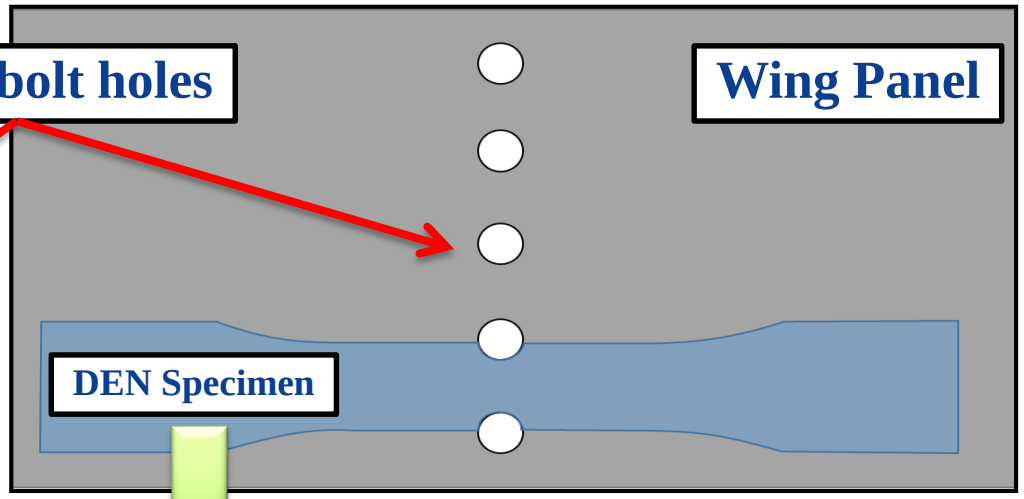
- Predictions using nominal geometry
  - All predicted crack path A-C-E
  - Predicted crack path for **3/30** specimens
- Modeling each **as-built geometry** resulted in correct crack path predictions for **29/30** specimens.



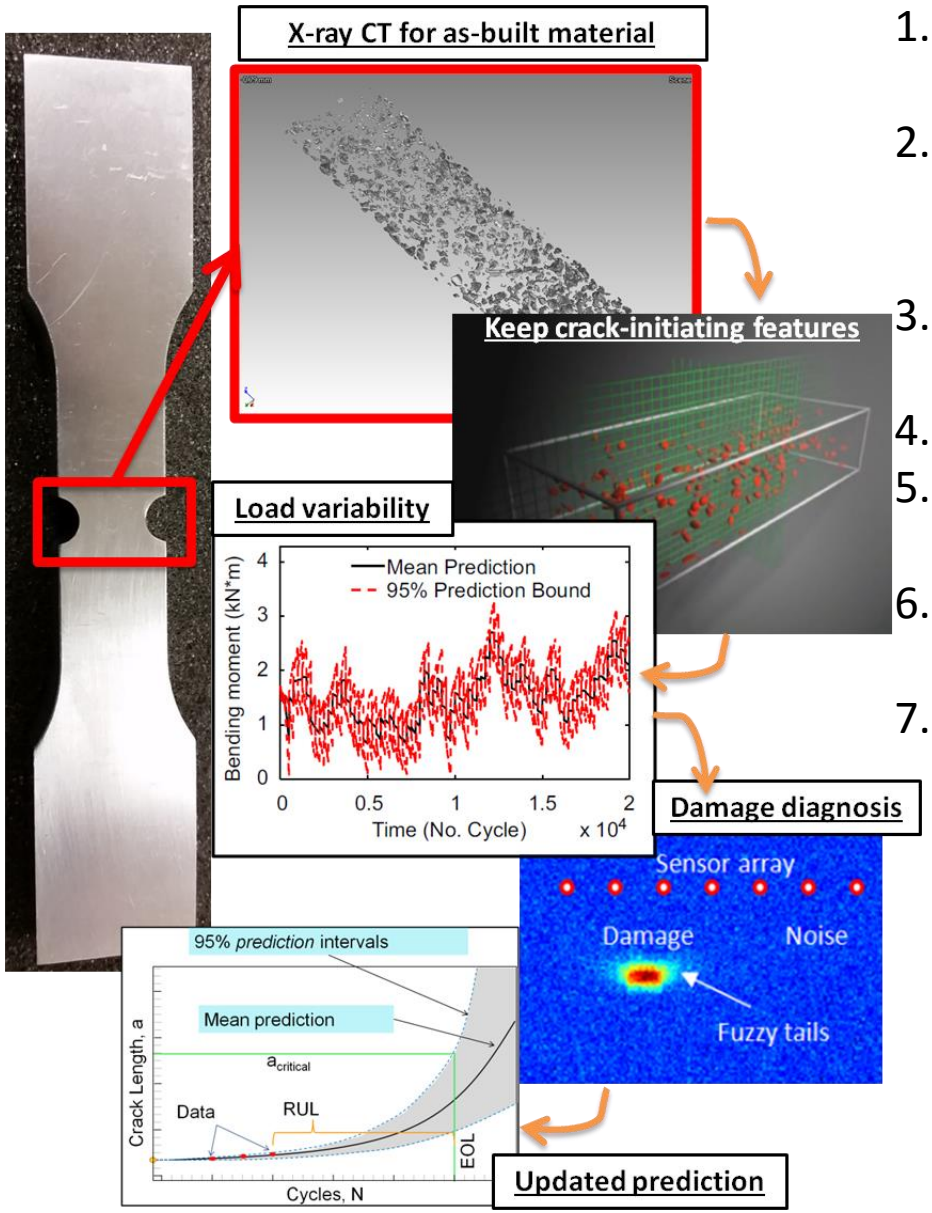
Virtual Flight Test

- "Fly" a double-edge notched (DEN) component to emulate a fatigue-critical component in service.
- Virtually "fly" digital twin of DEN
- Quantify the improvements and cost saving over existing methods.





Reducing Epistemic Uncertainty: Material



1. Complete X-ray CT analysis of DEN specimen to emulate a fatigue-critical component
2. Use advanced prognosis tools to predict at which microstructural features fatigue cracks will initiate under expected loading.
3. Apply load spectrum with random variations to introduce load uncertainties
4. Actively sense and diagnose any damage
5. Adaptively learn applied loads to better predict future load spectra
6. At the end of each "flight," update predictions based on actual usage and make next prognosis
7. Repeat steps 2-6 until failure occurs and answer:
   a) How accurate were we regarding crack growth throughout life?
   b) Were we able to predict the actual total life significantly earlier and more accurately than existing methods?
   c) Once we answer these 2 questions, can useful life be extended by altering usage?

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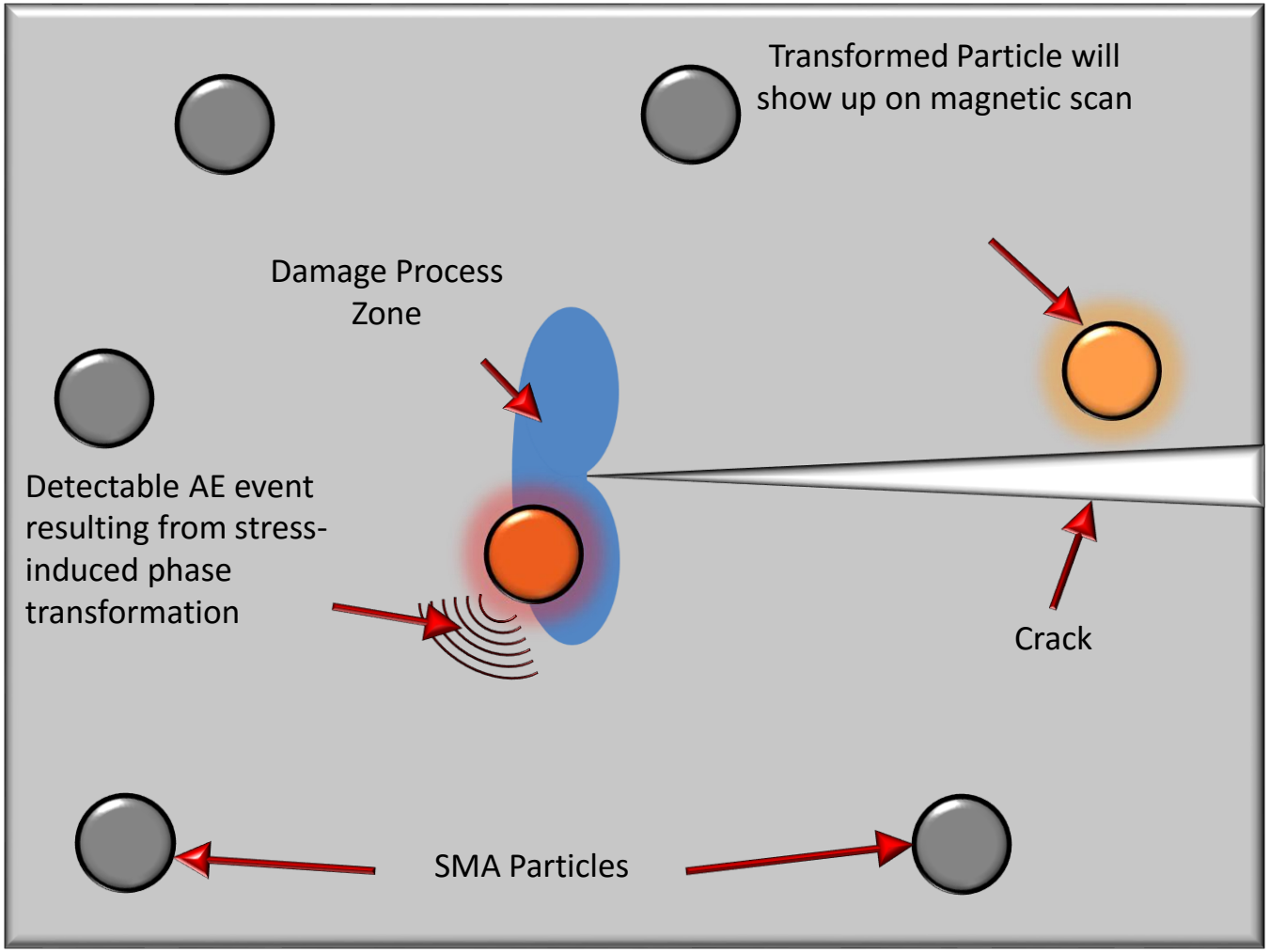
How can the digital twin get crack initiation updates from its physical twin in these early stages of crack growth?

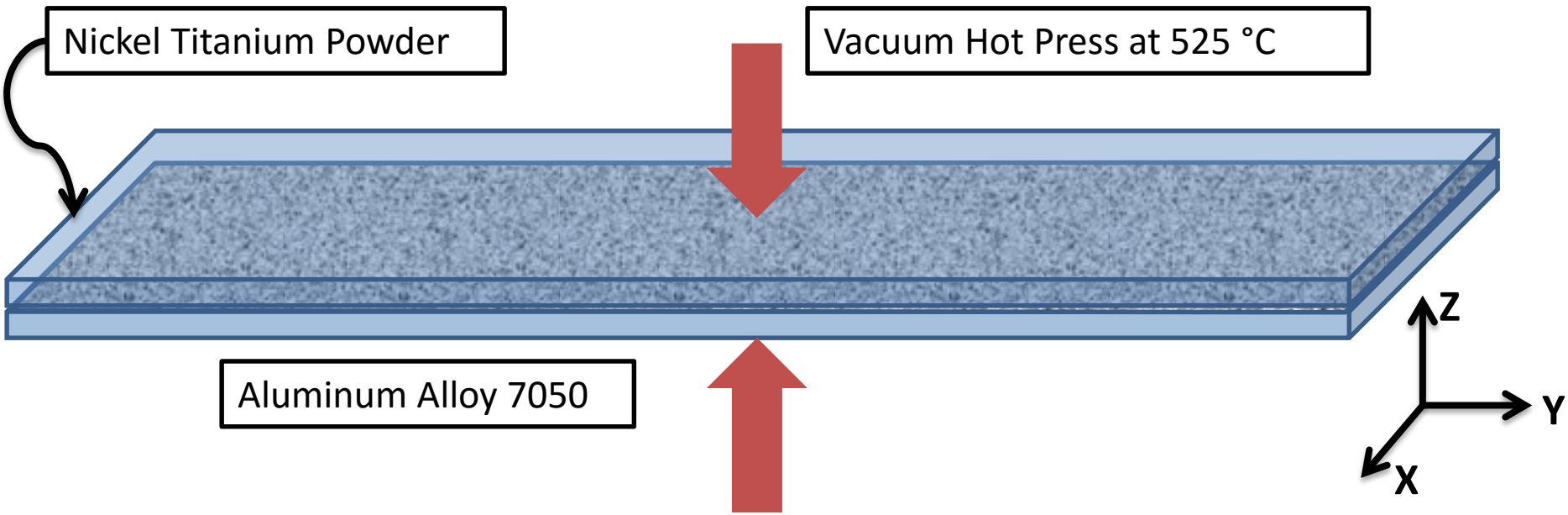
Traditional non-destructive evaluation methods will not work at that scale…

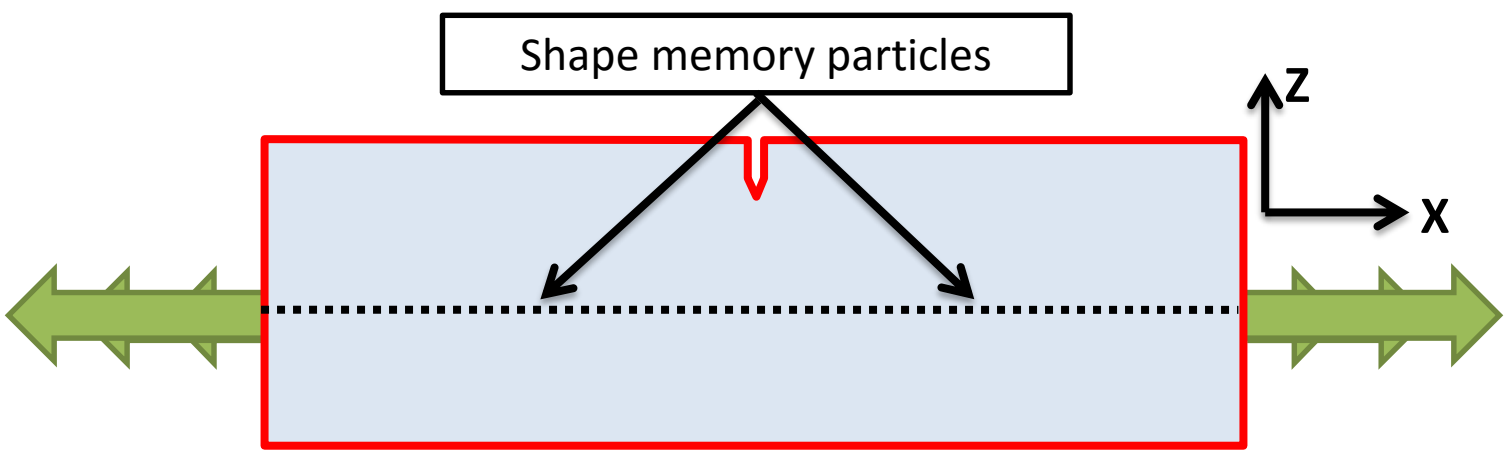
Sensory Particles*



*Wallace, T.A., Smith, S.W., Piascik, R.S., Horne, M.R., Messick, P.L., Alexa, J.A., Glaessgen, E.H. and Hailer, B.T., "Strain-Detecting Composite Materials". Patent Application Publication, Pub. No. 20100190026 A1, July 29, 2010.

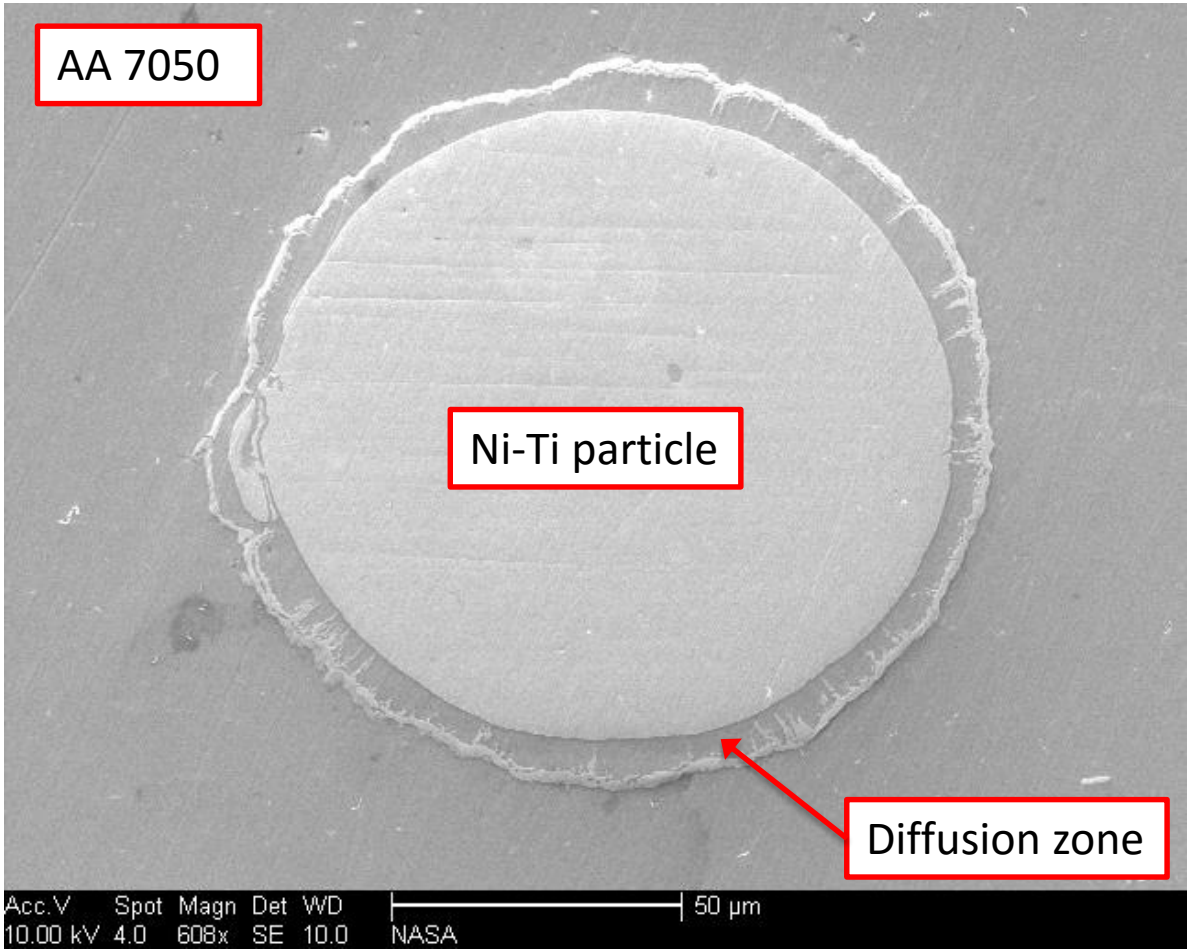
Sensory Particles: Fabrication



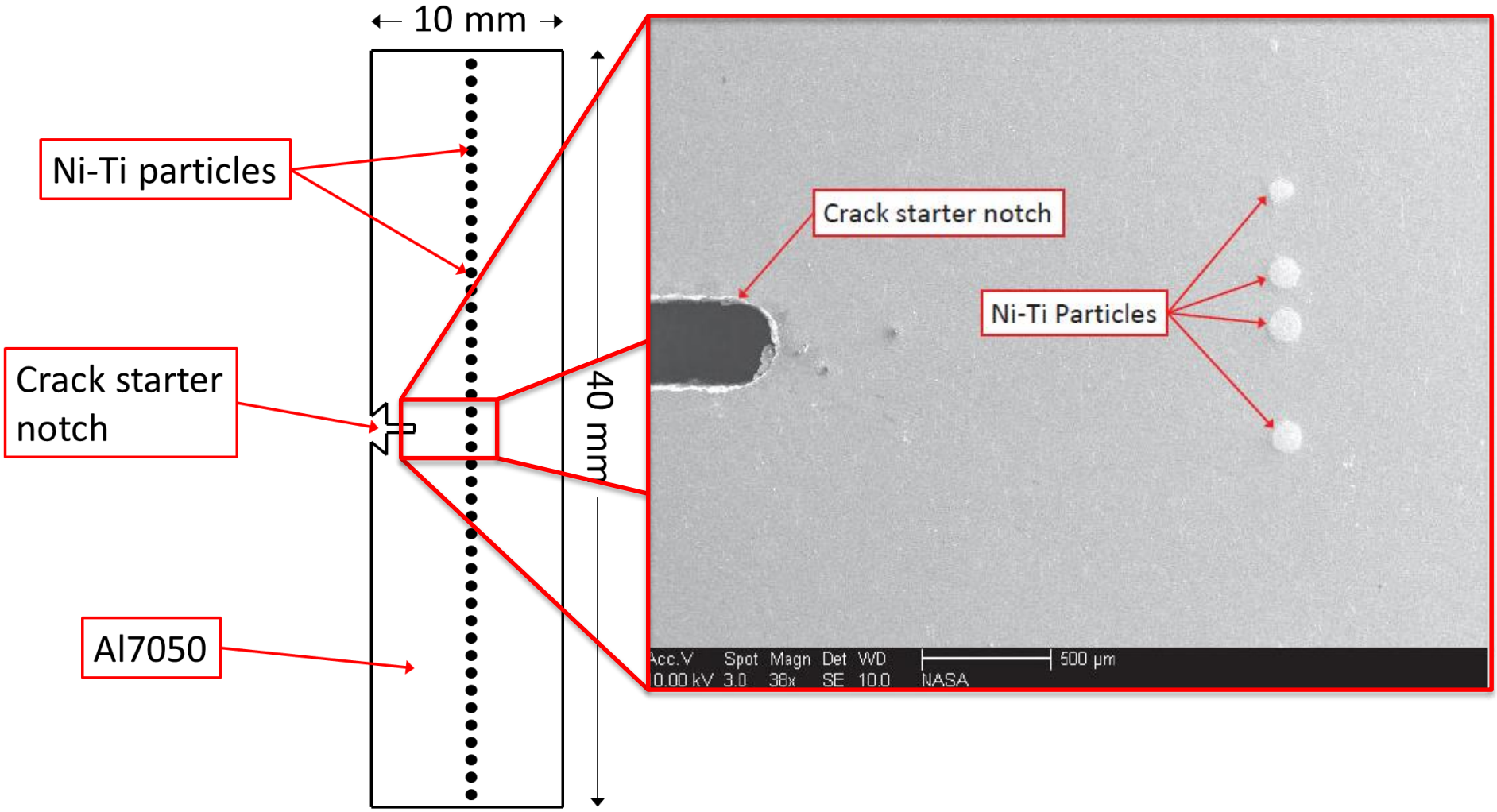


Heat Treatment – Ni-Ti

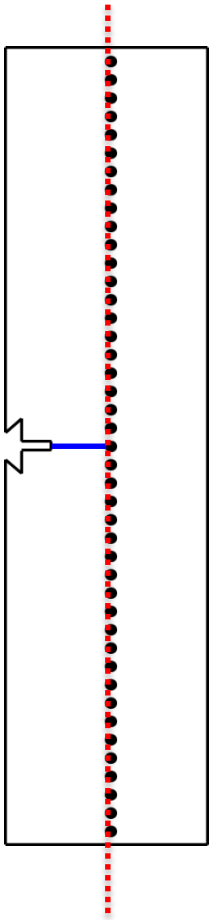
- Hot press
  - 525°C
- Solutionize
  - 490°C/6hr
  - Water quench
- Peak age
  - 121°C/24hr
  - Water quench
- Diffusion zone around particle reaches 5-10 microns

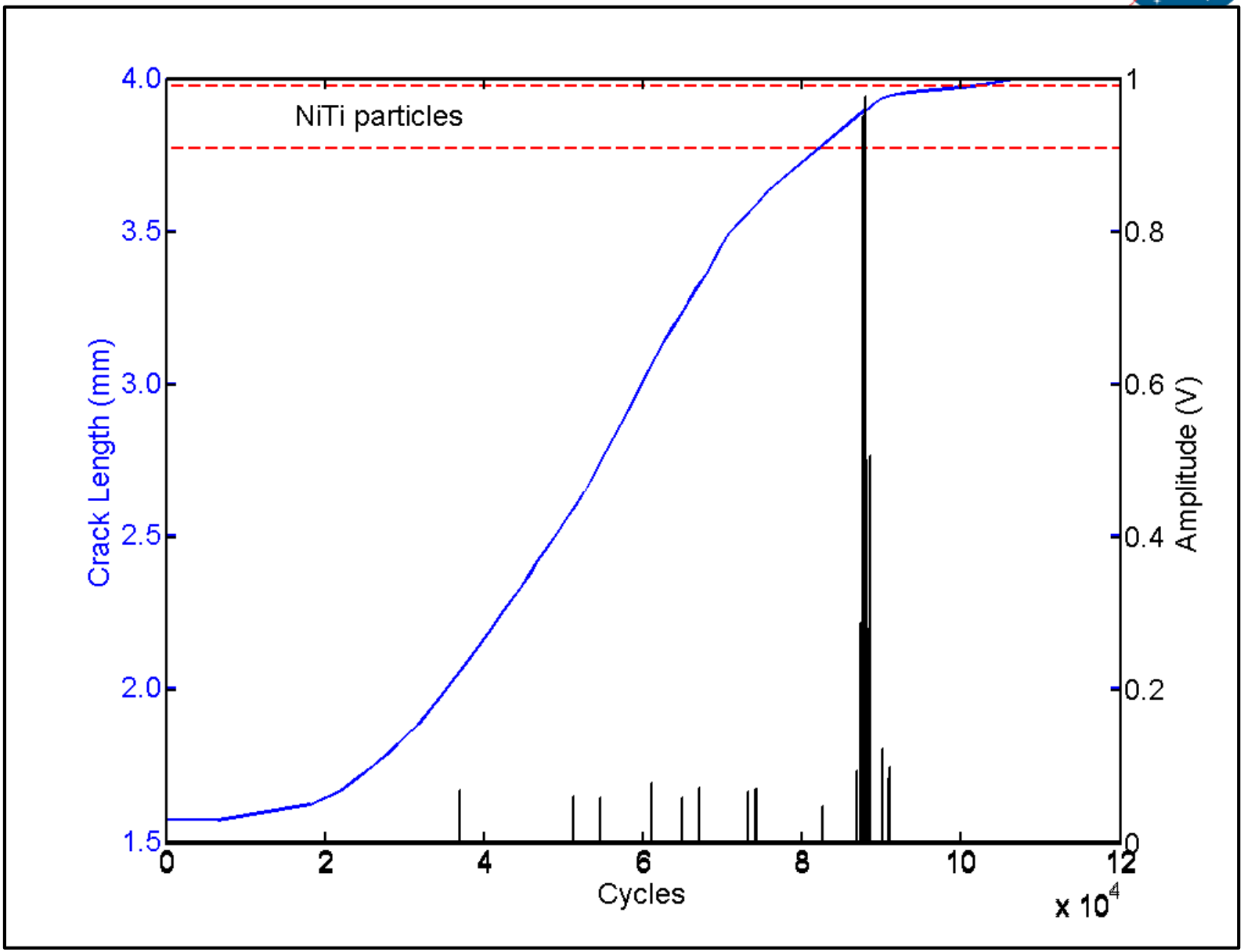


Specimen Example

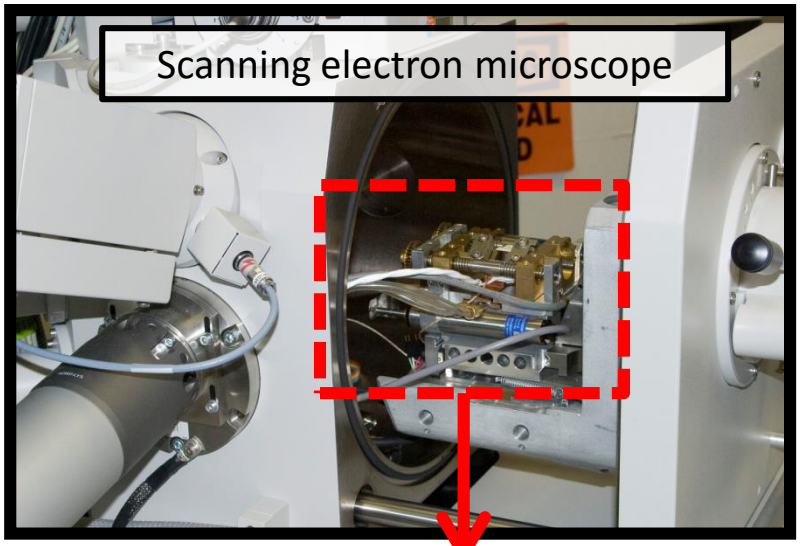


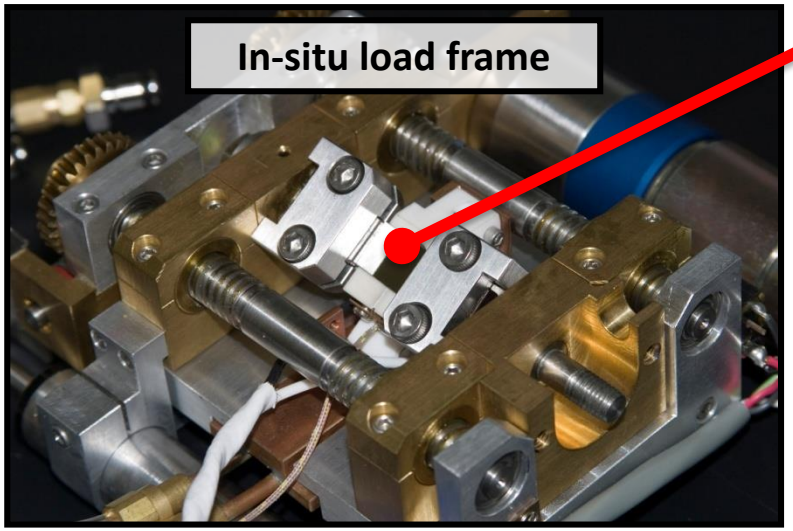
Fatigue Crack Growth



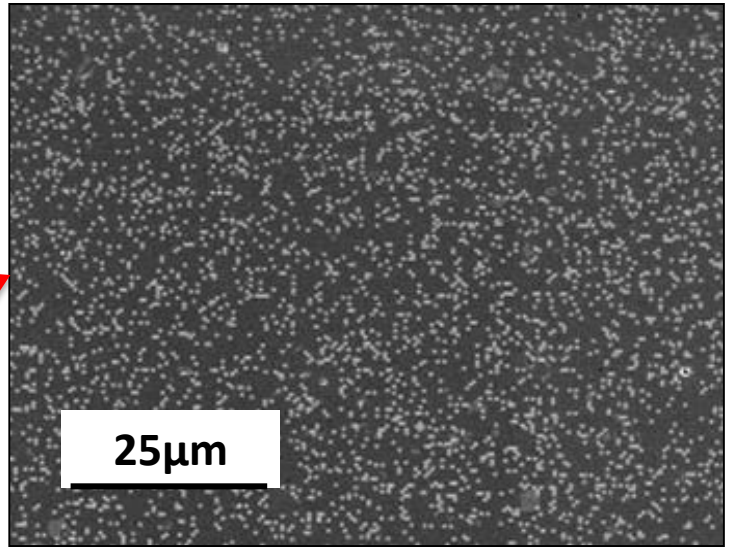


Micro-scale In-Situ Image Correlation



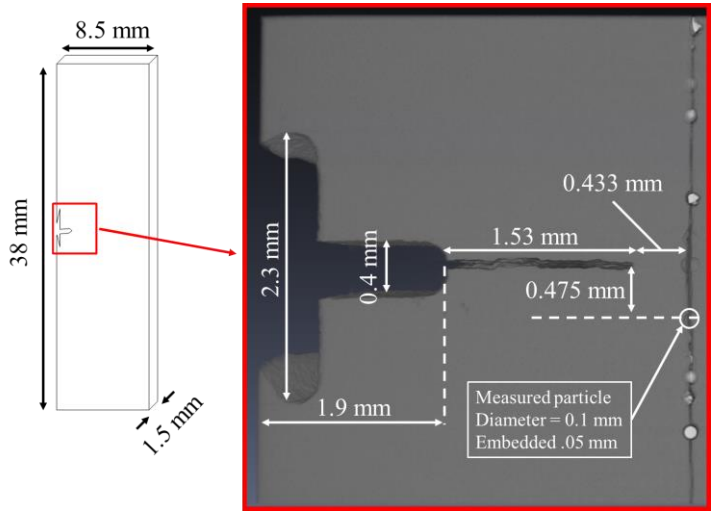


- Resolution < 2nm @ 7 Torr (FEG)
- Operating environment
  High Vacuum to 20 torr (H_2O, N_2)
- Temp. –20 to +1000 °C
- Tensile Stage, 4 kN, up to 1 Hz

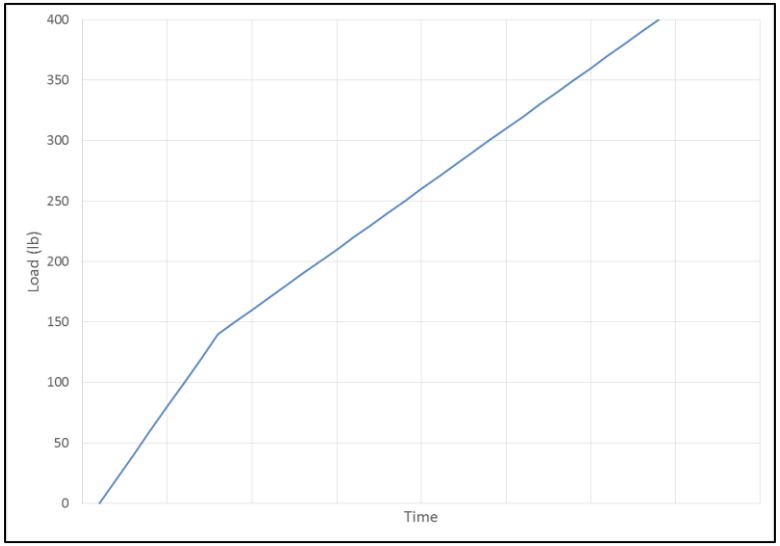


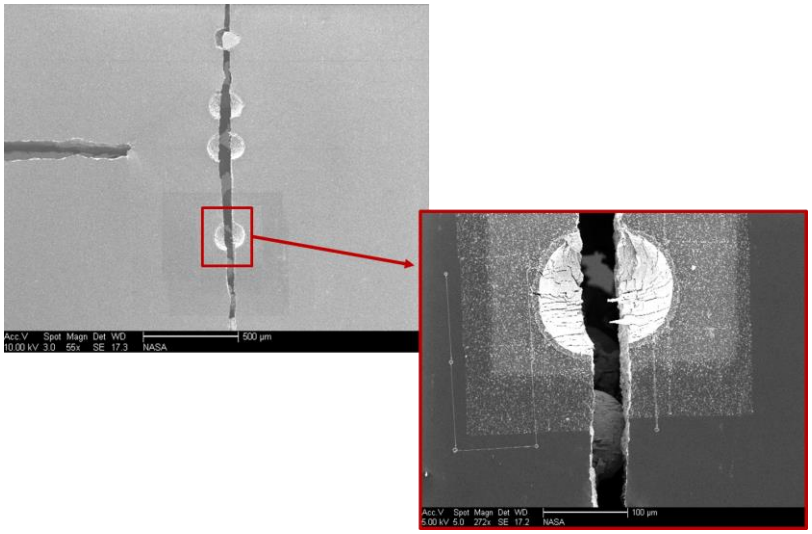
- e-beam lithography
- Base element ~150-5000 nm
- Microstructural effects on strain fields and cracking

Experiment



- NiTi particles hot-pressed between 2 Aluminum 7050 plates
- Loaded uniaxially to 400 lb_f, when the specimen fractured along the particle interface
- 2D SEM-DIC used to collect full-field strain data around the particle





Measuring the Strain Field

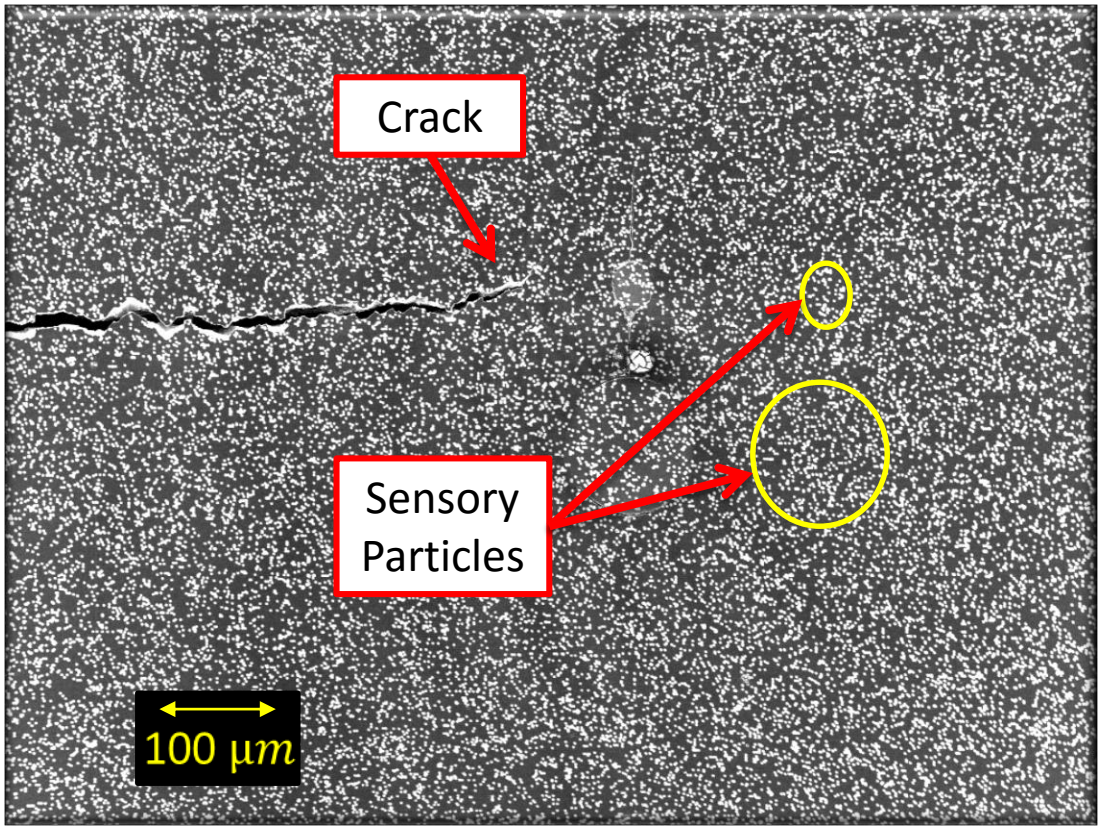
Specimen fatigue pre-cracked outside of ESEM

↓

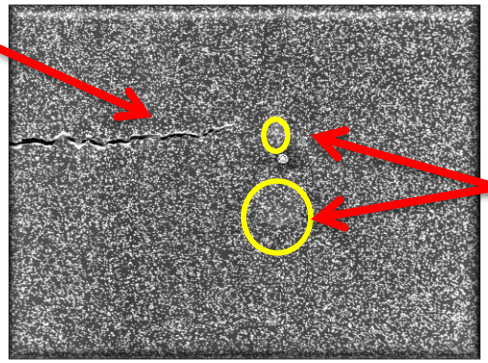
Patterned using e-beam lithography

↓

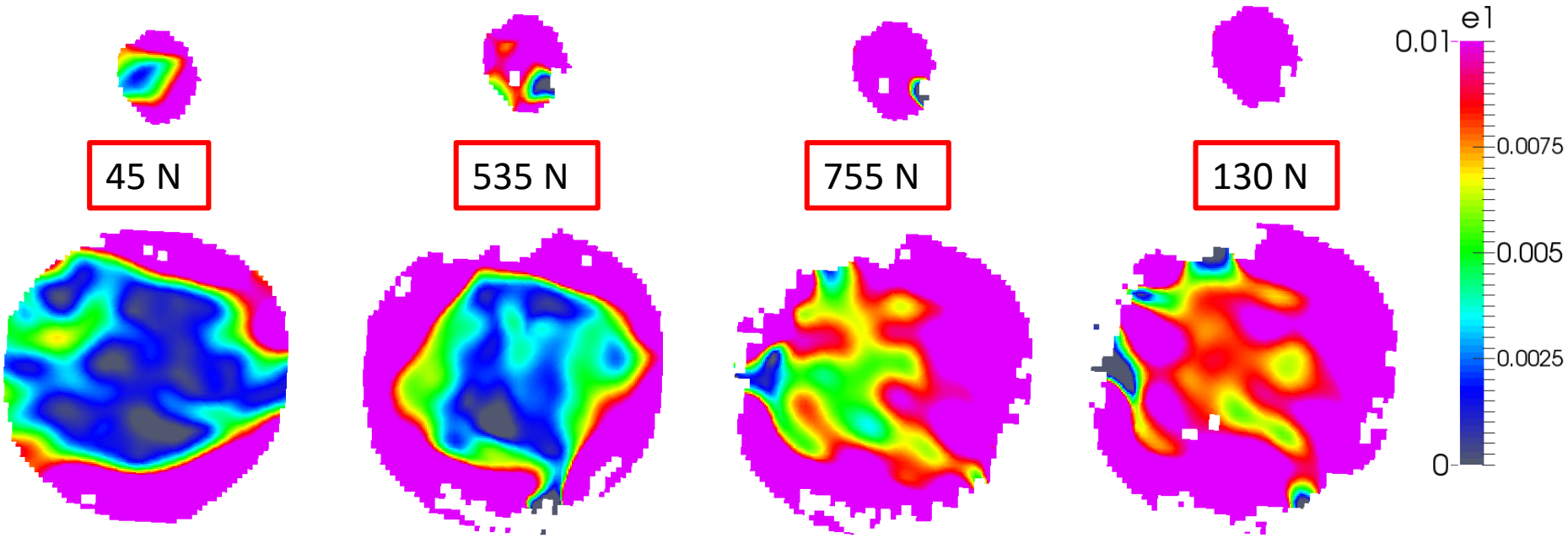
Loaded in ESEM



Strain Field Analysis

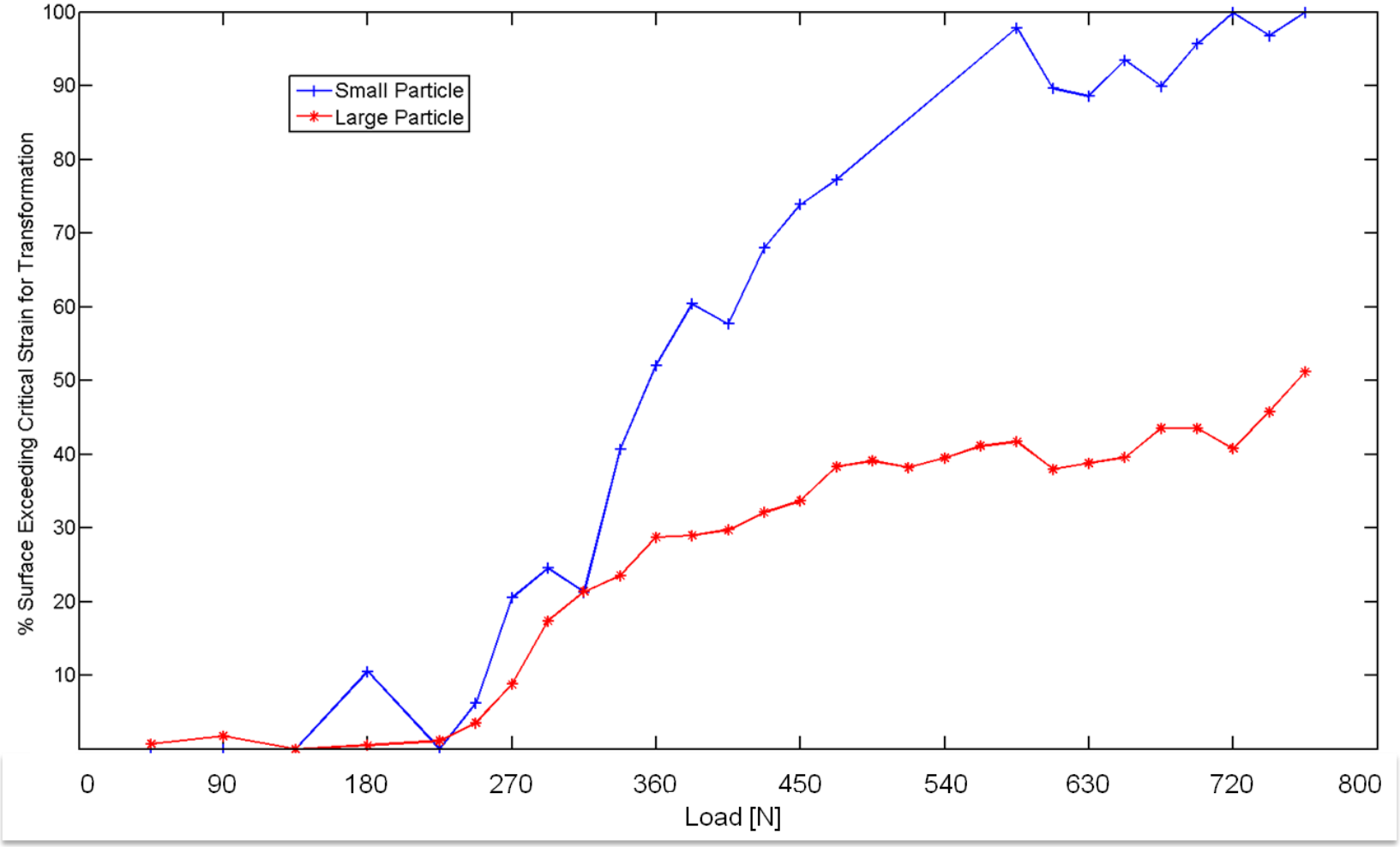


Purple regions have transformed

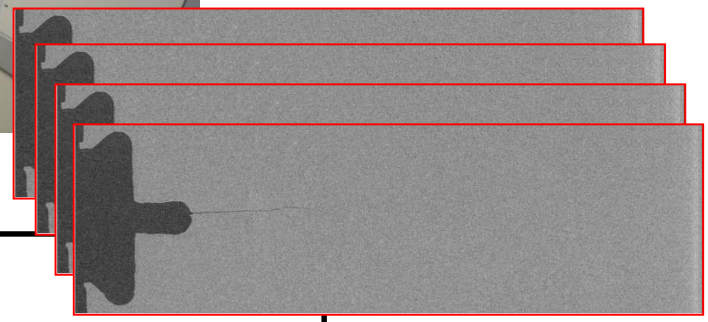


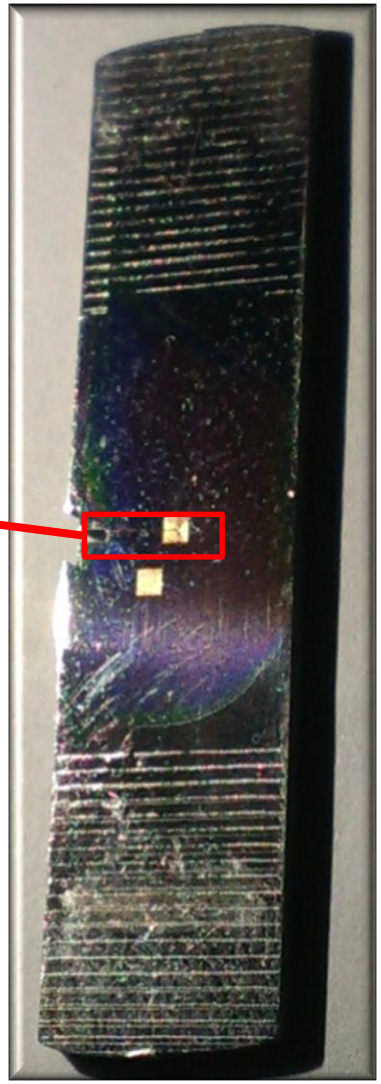
Particle Transformation Analysis

Much of the particle volume is transforming, maximizing the AE signal



X-Ray Micro-CT



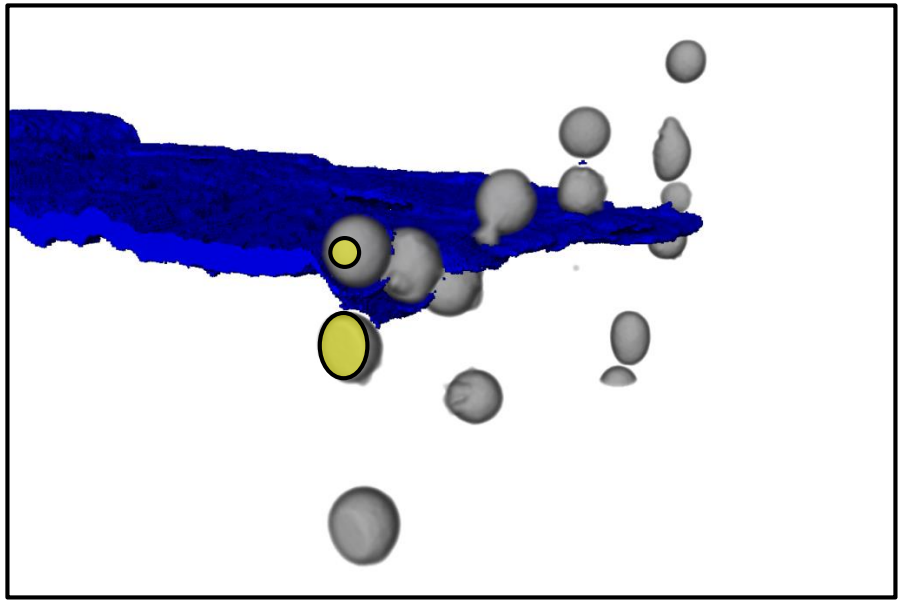


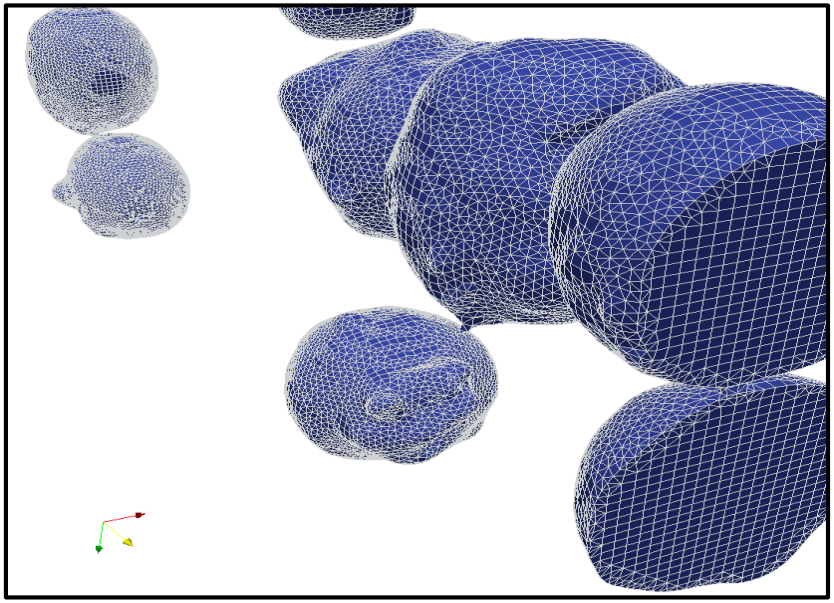
Specs of interest:

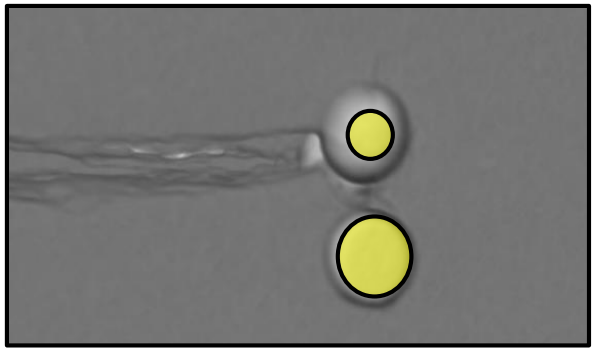
- X-Tek HMXST 225
- Voxel resolution of 3 μm
- Energy levels around 100 kV
- About 12 hours to scan a specimen

X-Ray Micro-CT Finite Element Analysis

- Cracks navigate around particles
- Detailed geometrical data for each sensory particle throughout volume



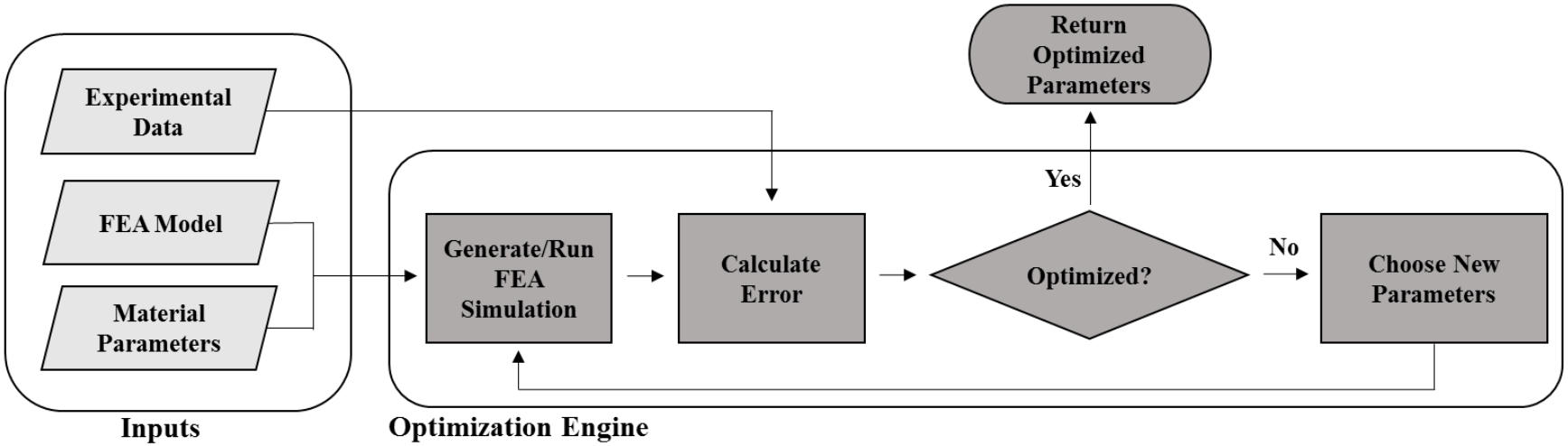




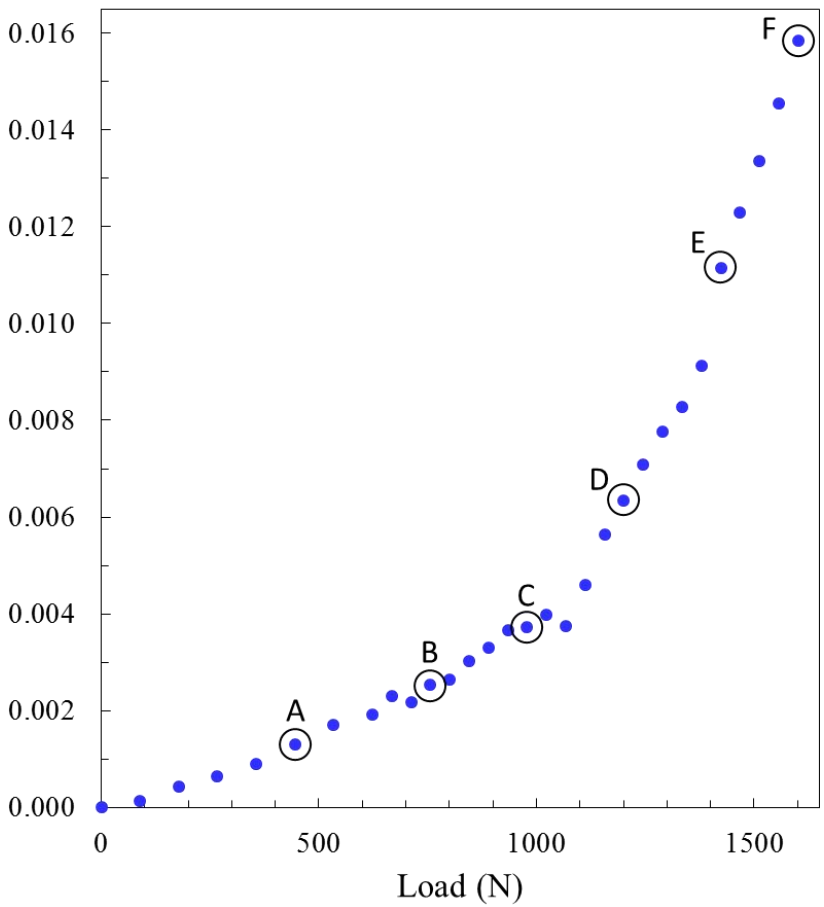
Optimization Framework

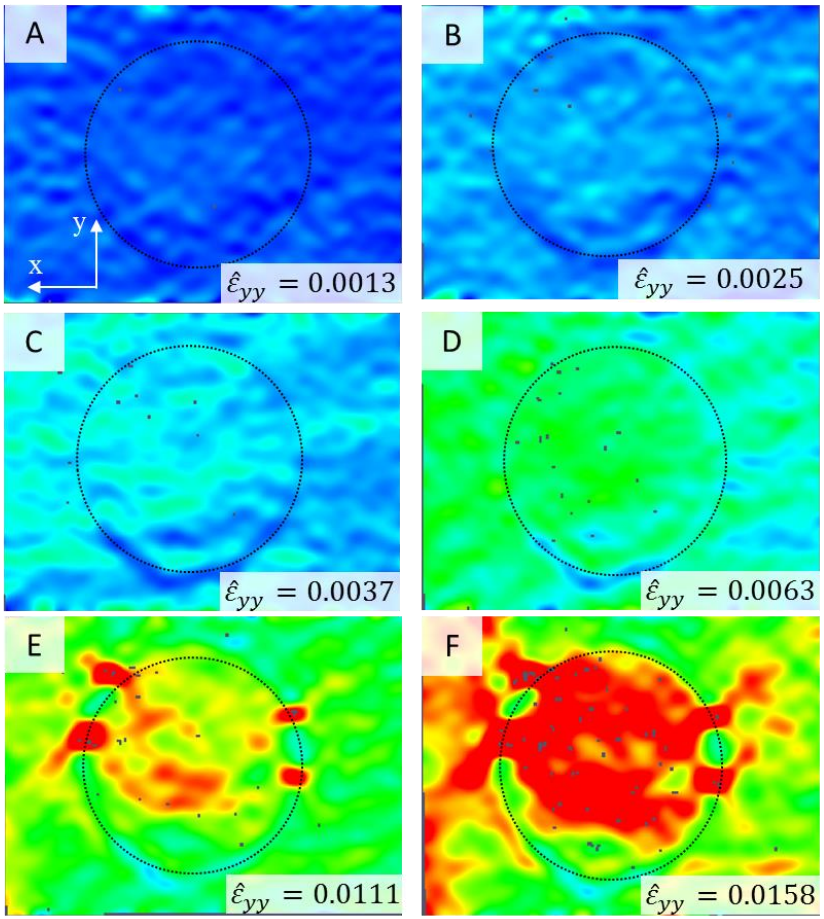
- The optimization engine uses Python scripts to integrate ABAQUS results with a variety of other program libraries
- SciPy optimization used to minimize the error between experimental data and simulated results

$$error = \sum (\varepsilon_{exp} - \varepsilon_{sim})^2$$

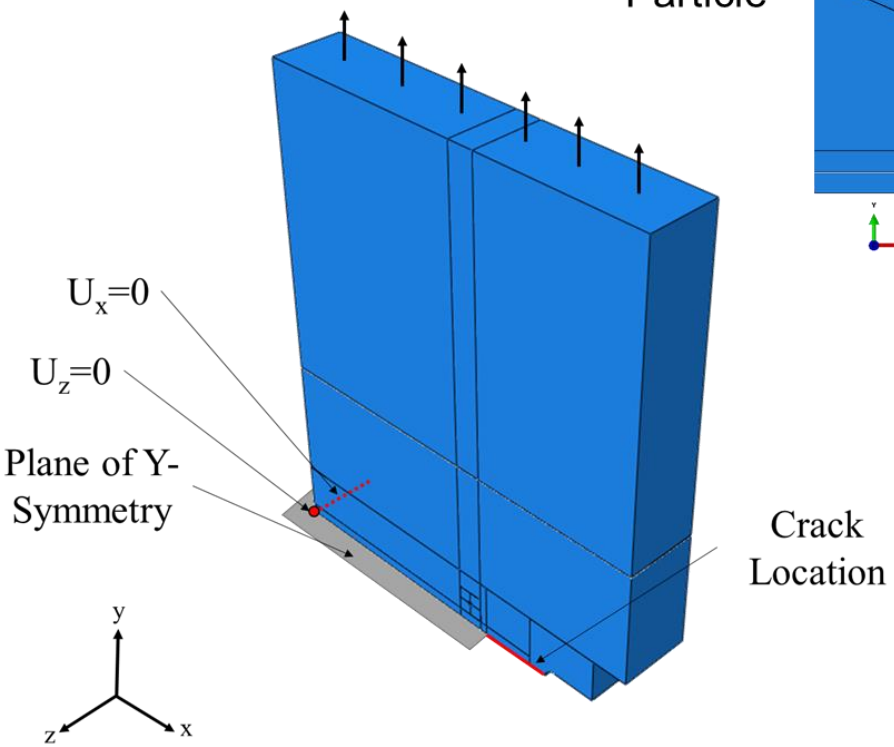


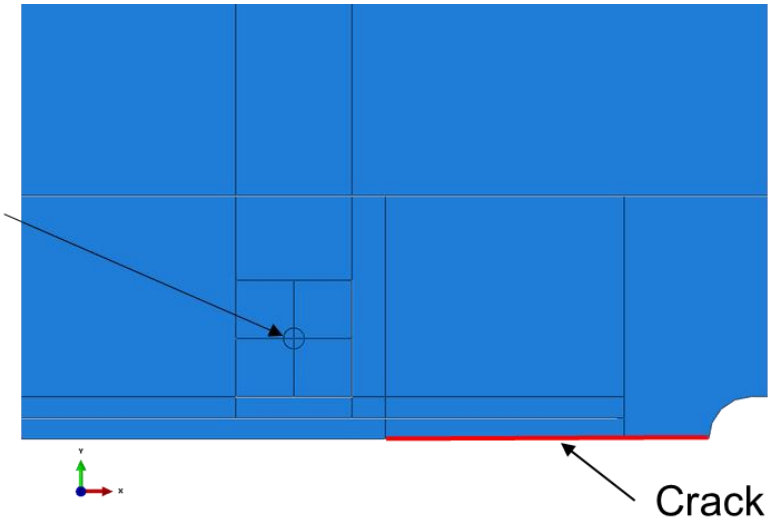
Experimental Data

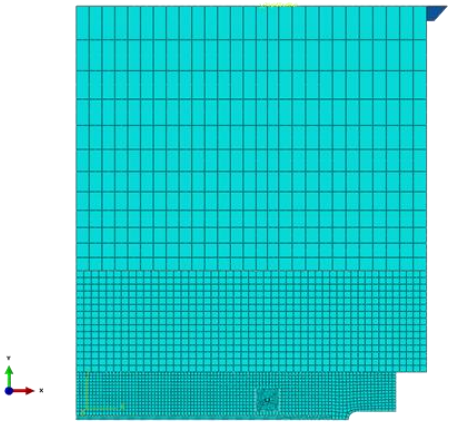




Finite Element Model

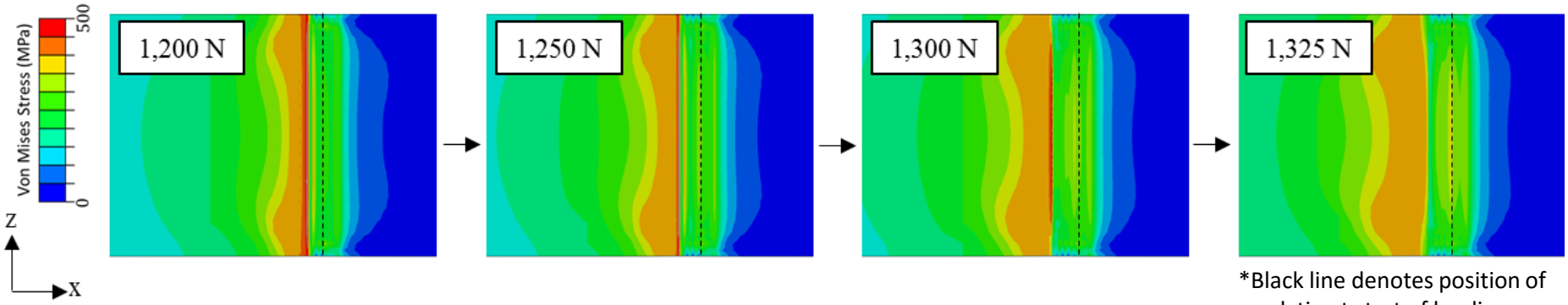






Modeling Crack Propagation

- No clear visual evidence as to the profile of the crack or rate of propagation during loading
- Approximated using a node-release technique, assuming we know the beginning and end of crack growth



*Black line denotes position of crack tip at start of loading

- Serves as a computationally efficient approximation for use in the optimization framework

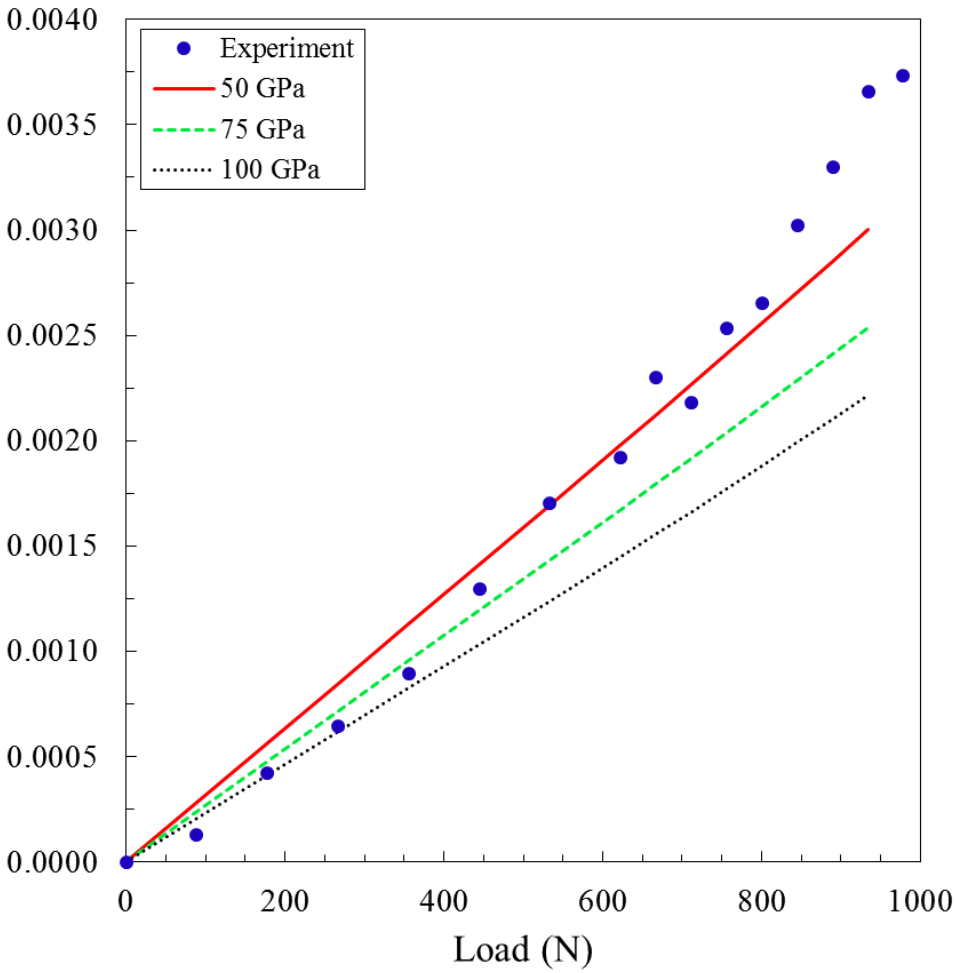
Material Parameters

Constant Parameters	
A_s	313 K
A_f	334 K
$\nu^M=\nu^A$	0.33
$C^M=C^A$	7.0 MPa/K
$n_1=n_2=n_3=n_4$	1.0

Optimized Parameters			
Parameter	**Lower Bound**	**Upper Bound**	**Initial Guess**
$E_A=E_M$ (GPa)	50	100	75
M_s (K)	258	295	278
M_f (K)	M_s - 35	M_s - 5	M_s - 15
H_{max} (%)	1.0	7.5	3.0

Elastic Calibration

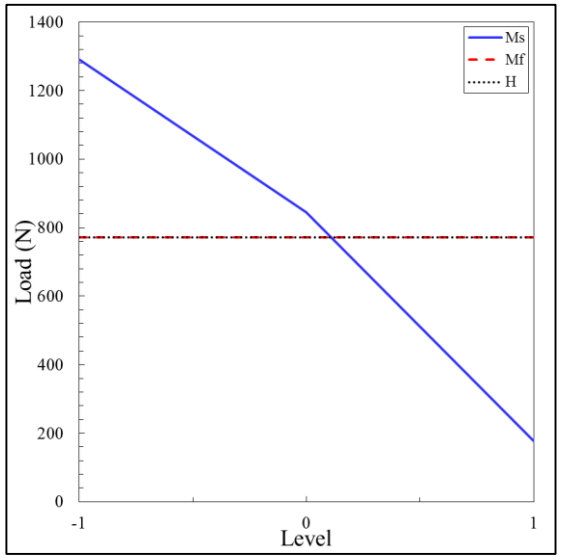
- Before optimization, the linear region of the experiment is considered
- Optimized parameters held to their initial values, E_A varied
- E_A=75 GPa determined to be the best match of the initial linear response (ie. up to a load of 500 N)



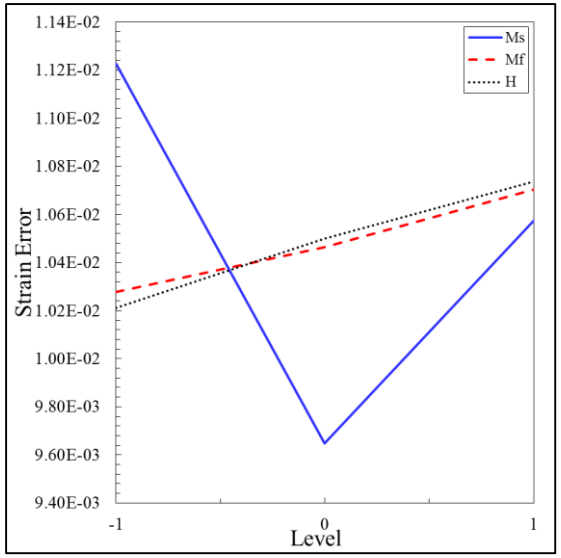
Material Property Trends

- Three-Level Full Factorial DOE Study conducted to quantify the effect of each parameter on particle response

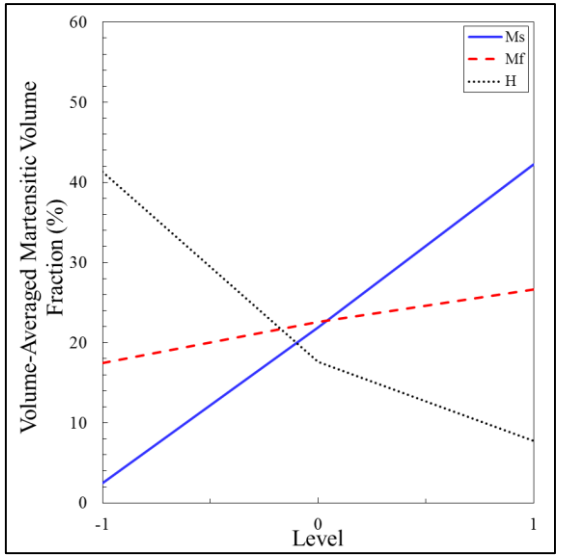
Level	M_s (K)	M_f (K)	H_{max} (%)
-1	258	M_s - 35	1.0
0	278	M_s - 15	3.0
1	295	M_s - 5	7.5



Load at which particle transformation initiates



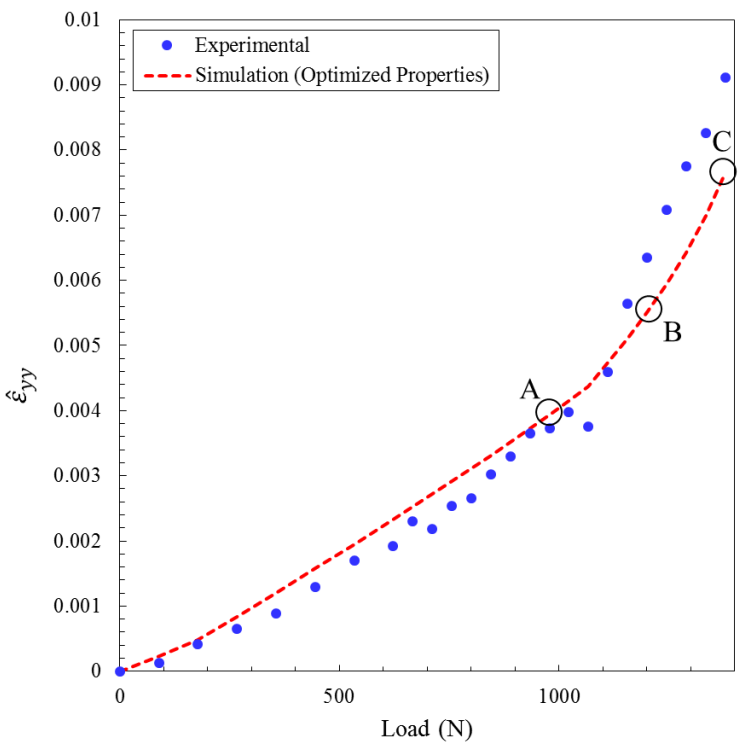
Error between experimental and simulated results

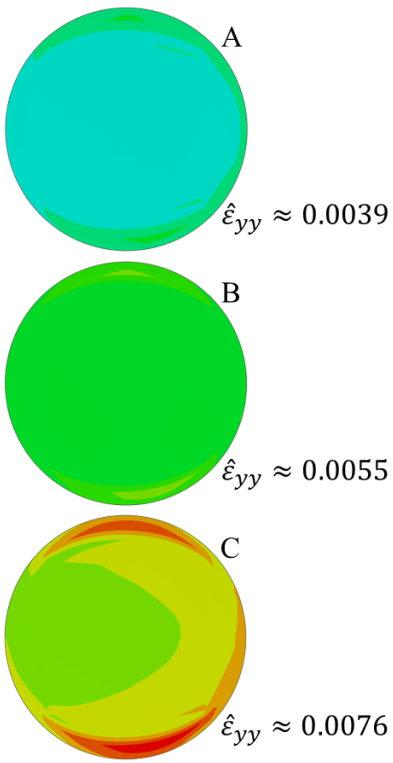


MVF of particle at end of loading

Optimization Results - Strain

Parameter	Lower Bound	Upper Bound	Initial Guess	Optimized
M_s (K)	258	295	278	292.8
M_f (K)	M_s - 35	M_s - 5	M_s - 15	258.3
H_{max} (%)	1.0	7.5	3.0	1.32





Optimization Results - MVF

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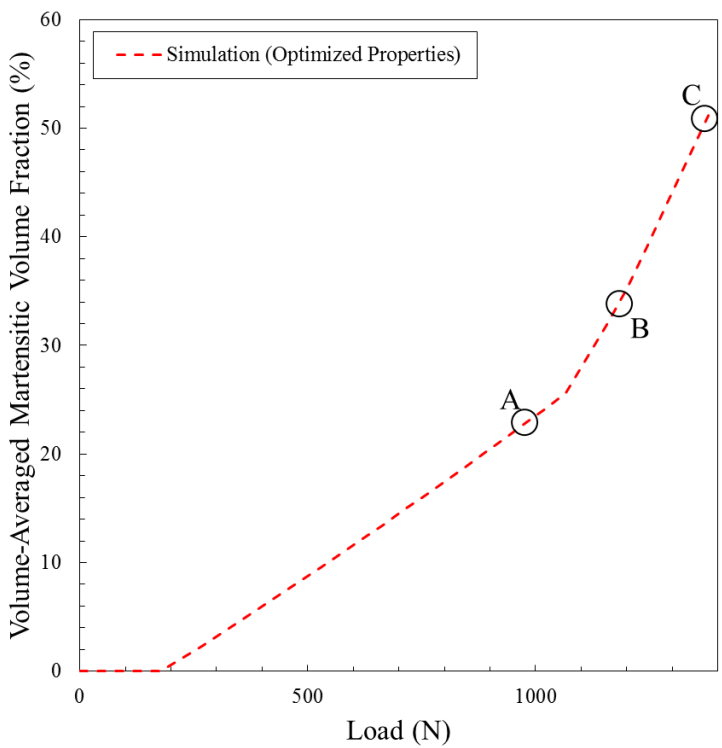
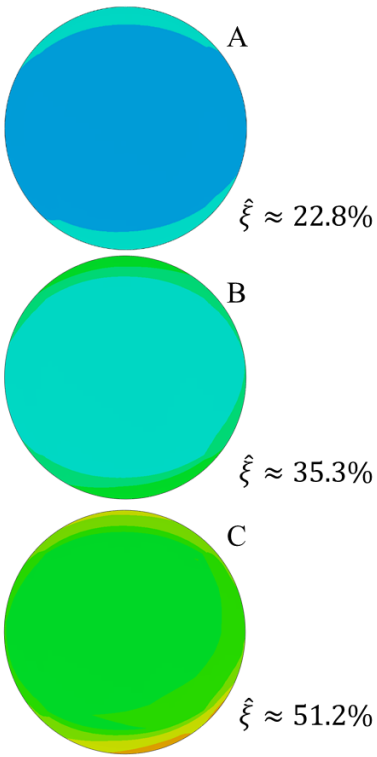
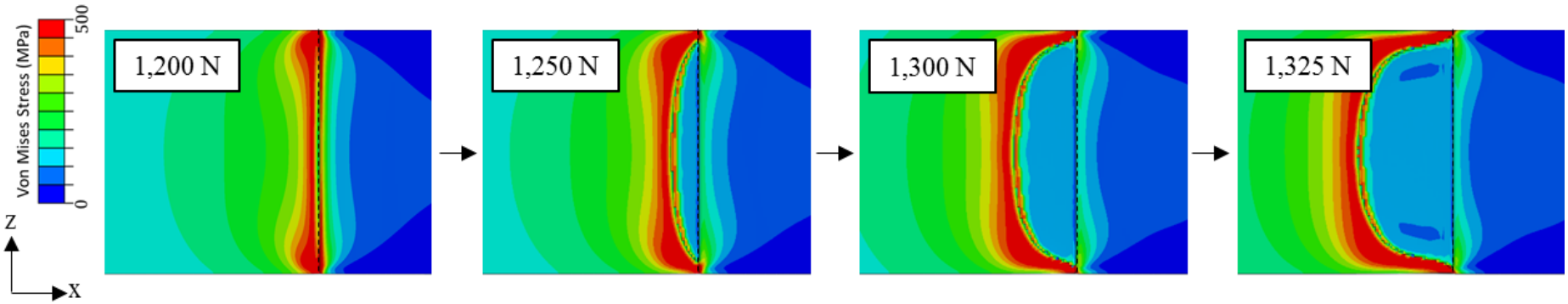




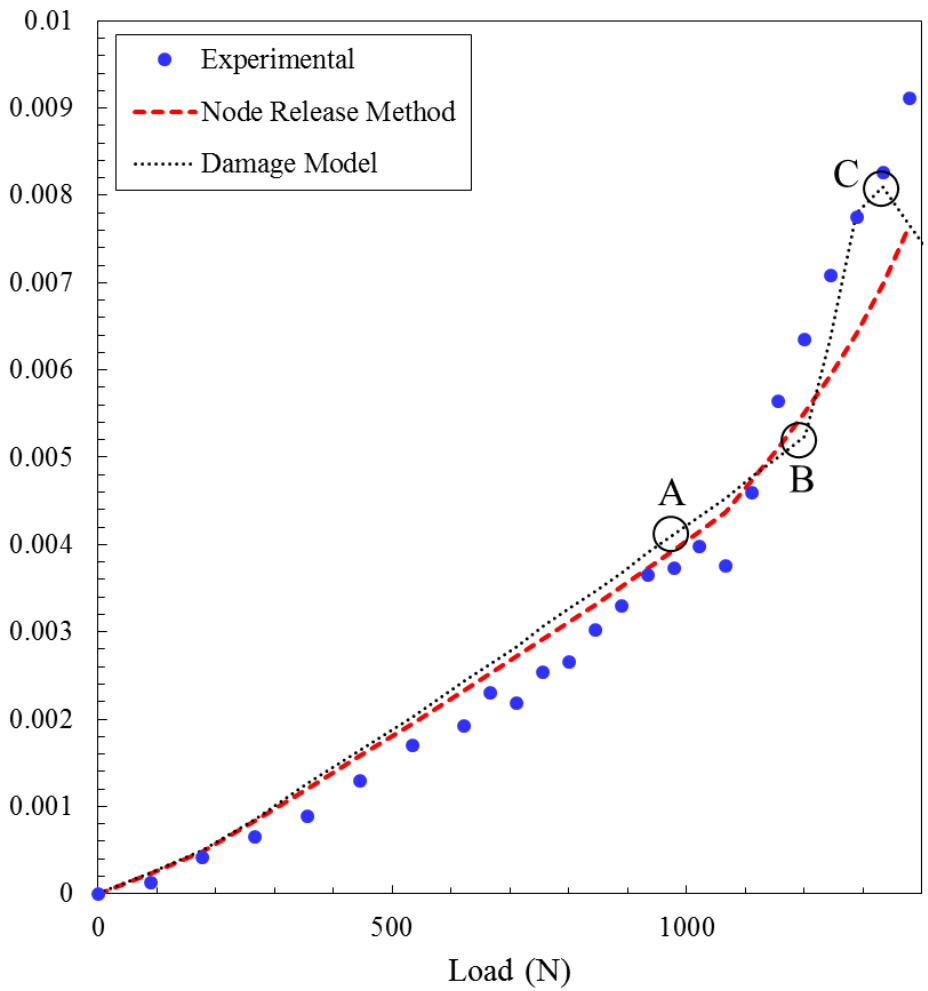
Damage Model

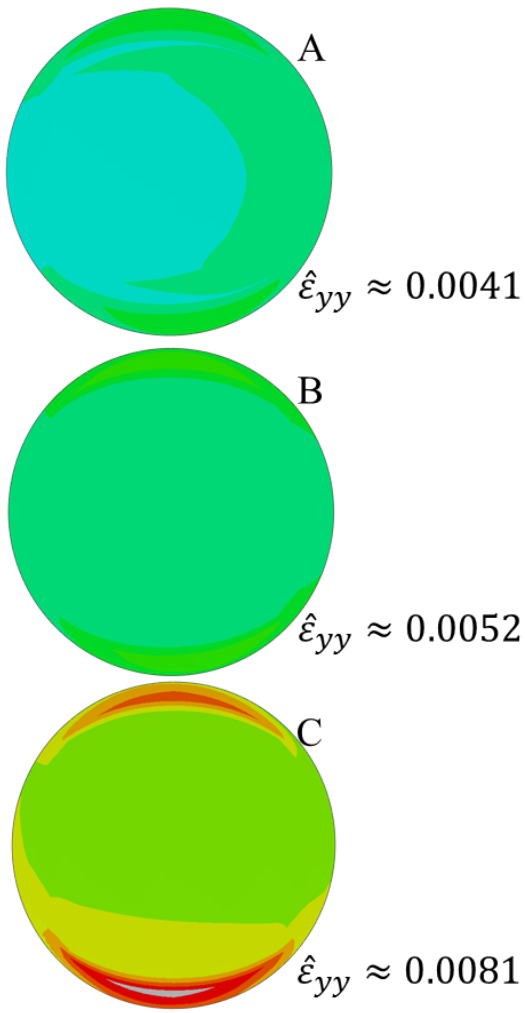
- To more rigorously simulate damage and potential crack propagation in the specimen, a ductile damage model was added to the FEA model
- Since data for damage calibration was not taken during the experiment, example data from a different aluminum system was used



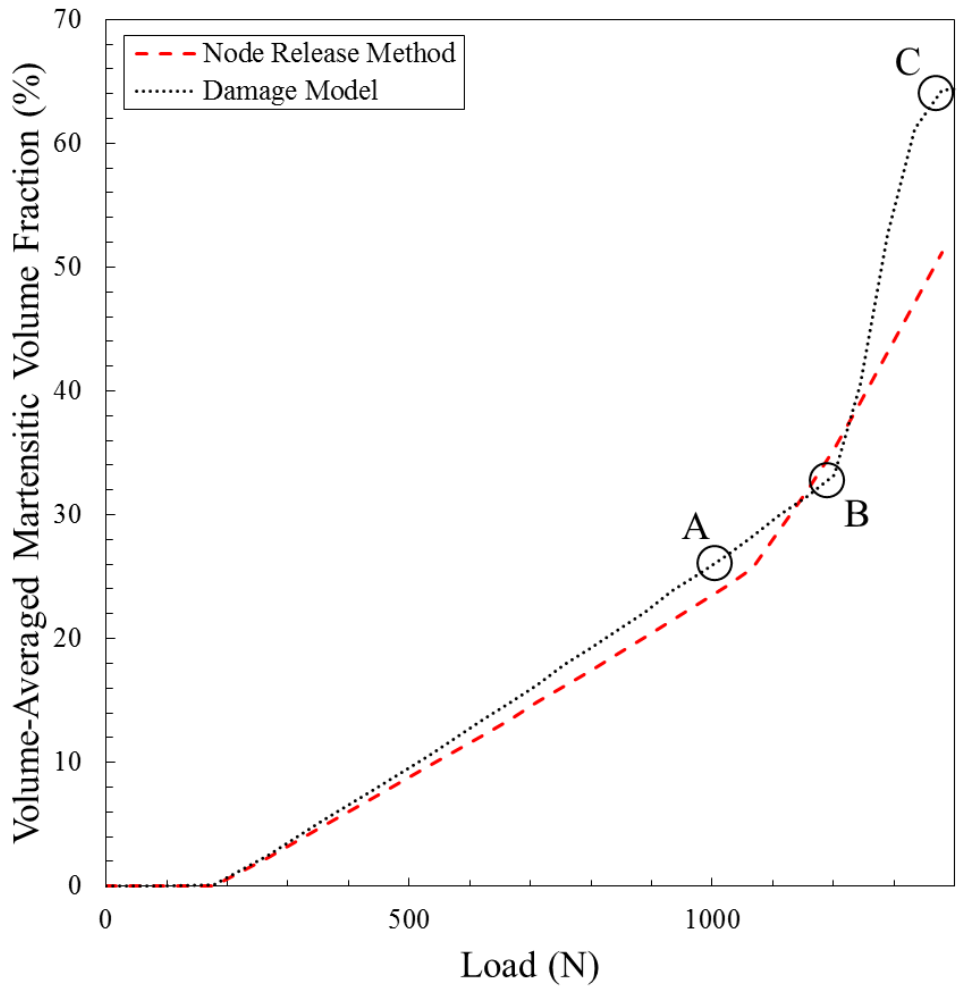
- Damage model predicts crack growth initiation after what was seen in the experiment and growth past the particle interface before the experiment
- However, damage model predicts a crack profile more representative of what has been observed during experimental testing of ductile materals (ie. crack tunneling)

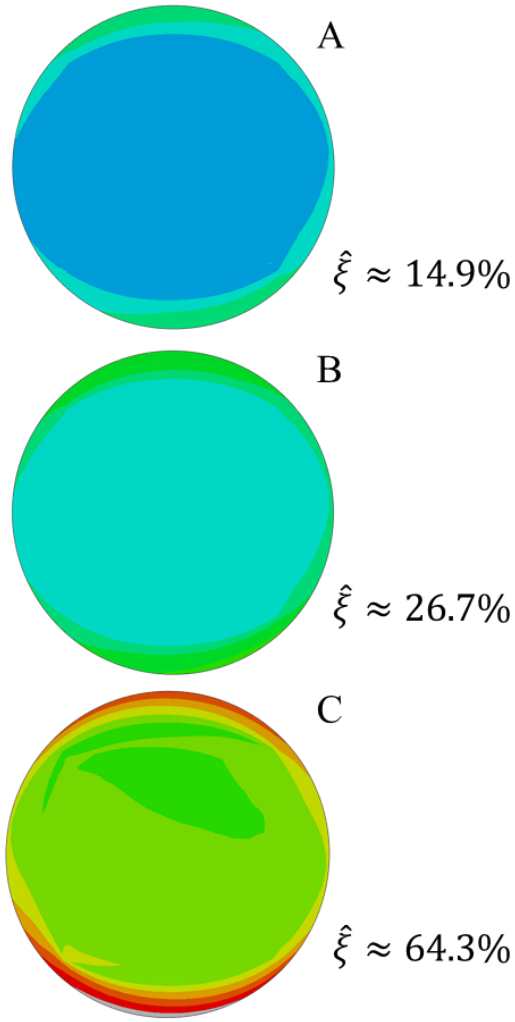
Damage Model Results - Strain





Damage Model Results - MVF



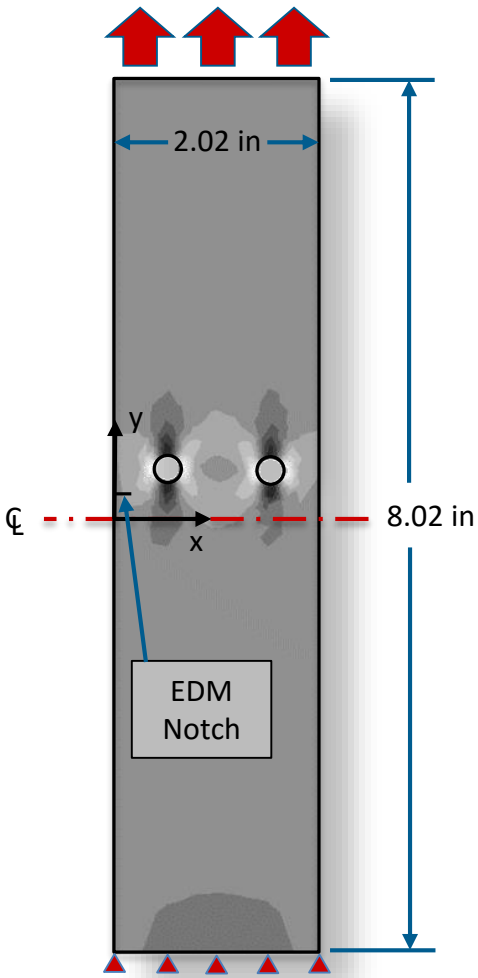


Outline

- Uncertainty, and what it means for design, certification, and maintenance standards
- Digital Twin
  - Concept
  - Geometric and Material Uncertainties
- Sensory Particles
- Encompassing Example
- Other Related and Requisite Technology
- Summary

Experimental Validation

Specimen design and experimental setup

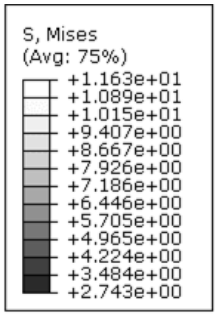


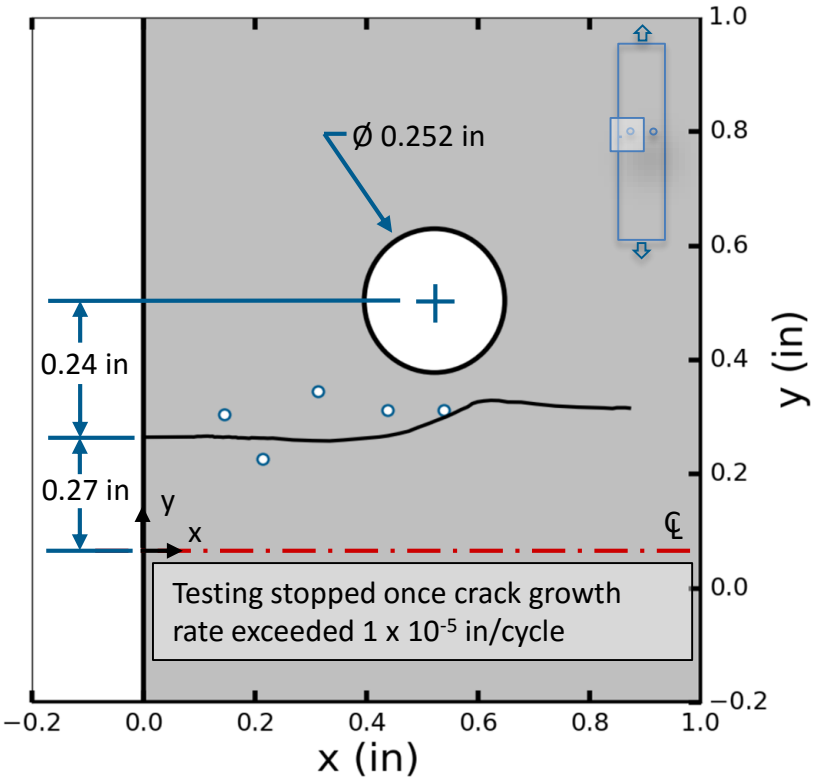
Material: AA2024-T3
Tension-tension fatigue
Constant amplitude stress: 5.95 ksi
Frequency: 10 Hz
Load ratio, R: 0.1

Thickness: 0.0805 in
Notch Length: 0.0815 in

Gaussian white noise , $N(0, \sigma^2)$, added to the *x,y* visual measurements with variances:

- $\sigma_x^2 = 0.0004$ in^2
- $\sigma_y^2 = 0.0020$ in^2





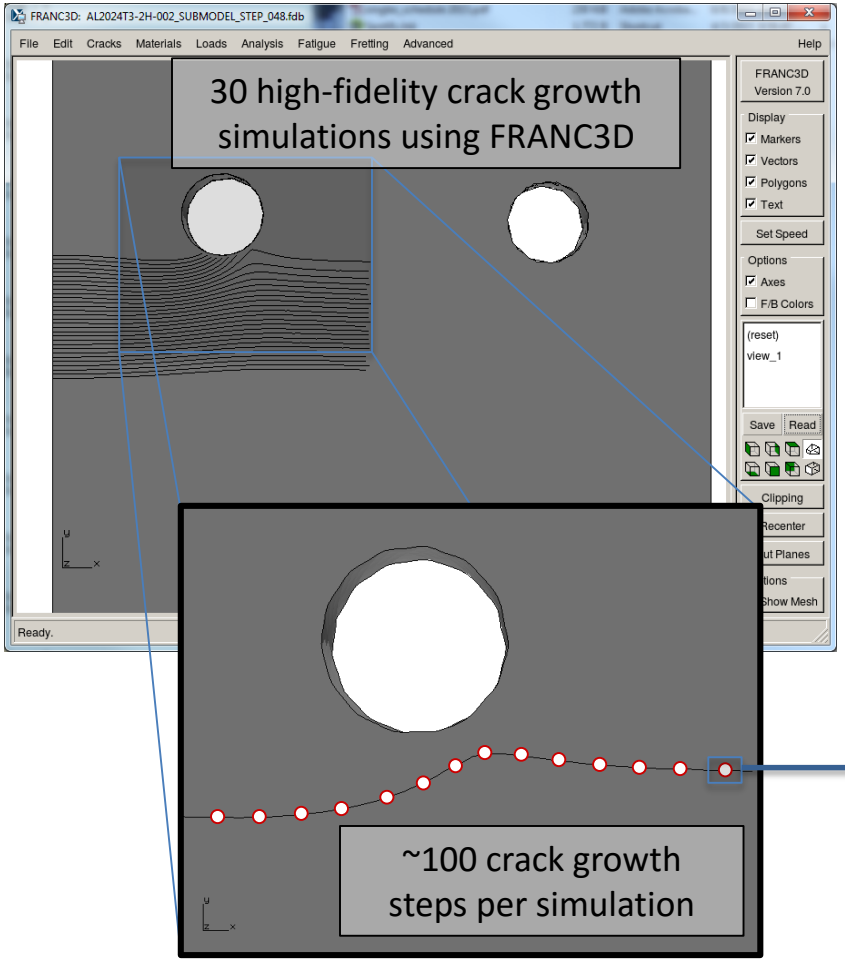
LEGEND

Observed crack path (experiment)

Visual data (noise added)

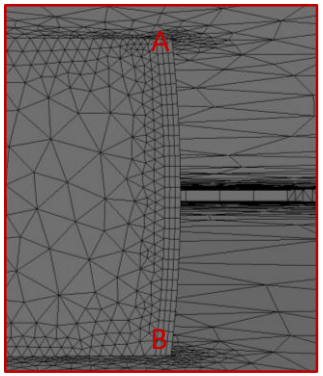
Experimental Validation

Obtaining training data for the surrogate model

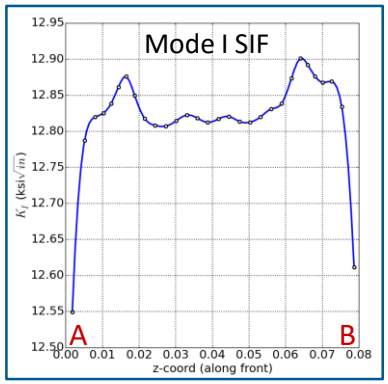


- *INPUTS*:
  - 3D representation of the crack front
- *OUTPUTS*:
  - Stress intensity factors, *K*, along the crack front

$$30\ simulations\ \times \sim 100\ growth\ steps\ \approx 3{,}000\ data\ points$$



Crack front (top view)

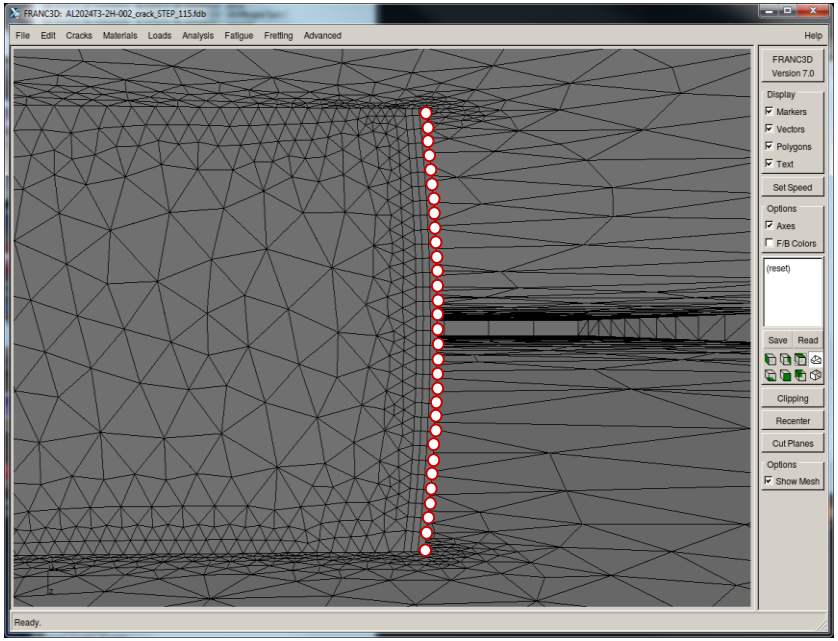


SIF profile

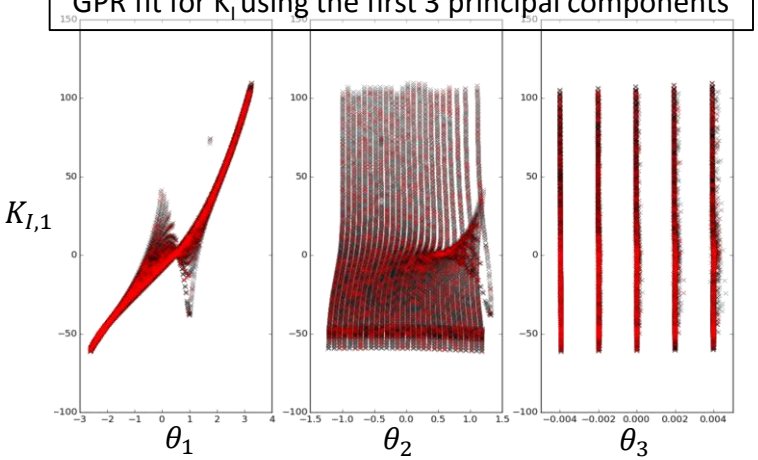
Experimental Validation

Training procedure for the surrogate model

- Dimensionally reduce the 3D crack fronts via principal component analysis (PCA)
  1. Standardize front dimension
  2. Obtain principal components
  3. Retain necessary number of components
- Fit the resulting reduced parameter space to corresponding *K* values using Gaussian process regression (GPR)[1]



GPR fit for K_I using the first 3 principal components



$$\sim 30\ front\ points\ \times 3\ axes \approx 90\ crack\ front\ parameters$$

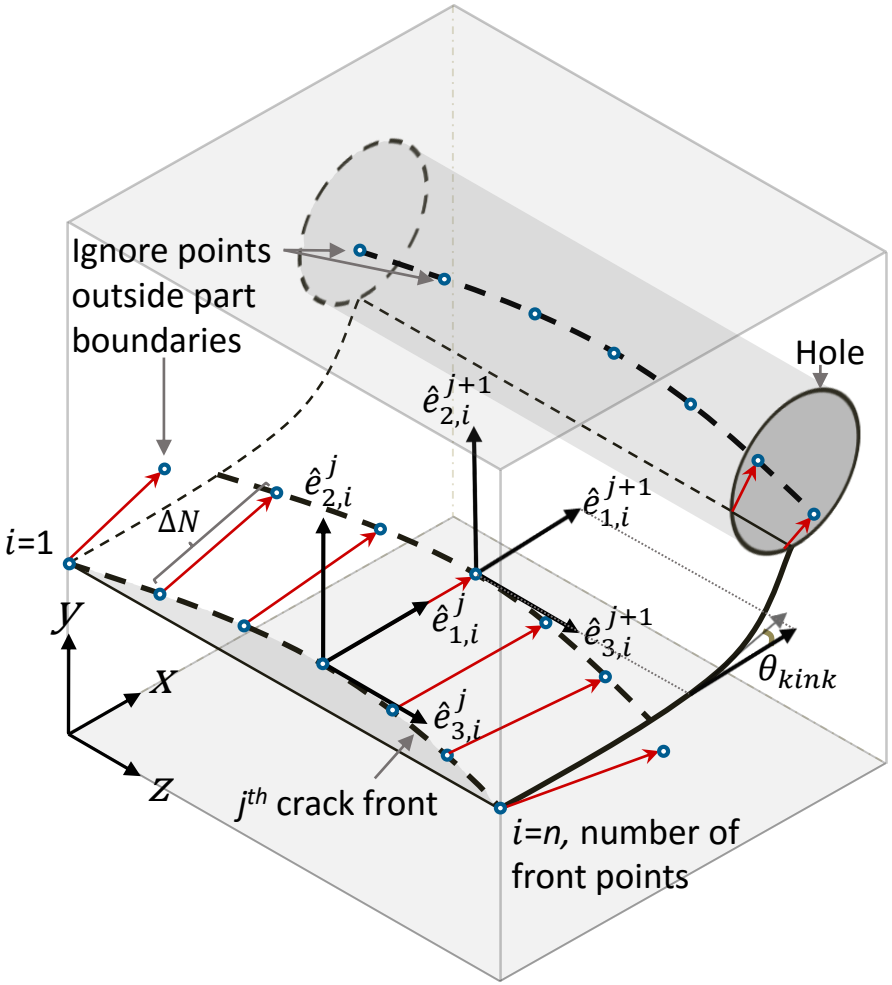
PCA

Reduces to 2-4 parameters while still accounting for ≥ 99% of the variance in the original dataset

1. Used Python module Scikit-learn which is documented in: Pedregosa, F., G. Varoquaux, and A. Gramfort. 2011. "Scikit-learn: Machine learning in Python," *The Journal of Machine Learning Research*, 12:2825-2830.

Experimental Validation

Growth algorithm



- Initialize crack front geometry (represented as points in space)
- Use surrogate model to obtain SIFs for each point
- Calculate kink angle/growth vector at each point
- Growth rate equation (e.g., Paris' Law) dictates magnitude of growth vectors based on a prescribed number of cycles
- Project forward to obtain new crack front, use surrogate to obtain SIFs

$K > K_{EOL}$

No

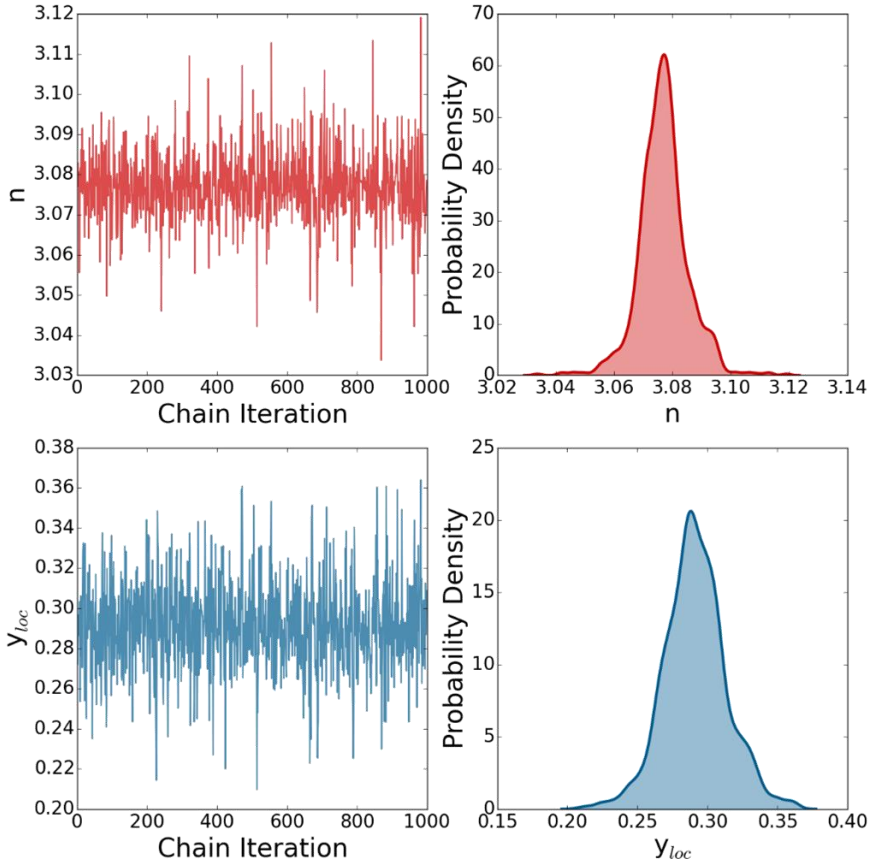
Yes

Store growth history and cycle count at end of life (EOL)

Experimental Validation

Results

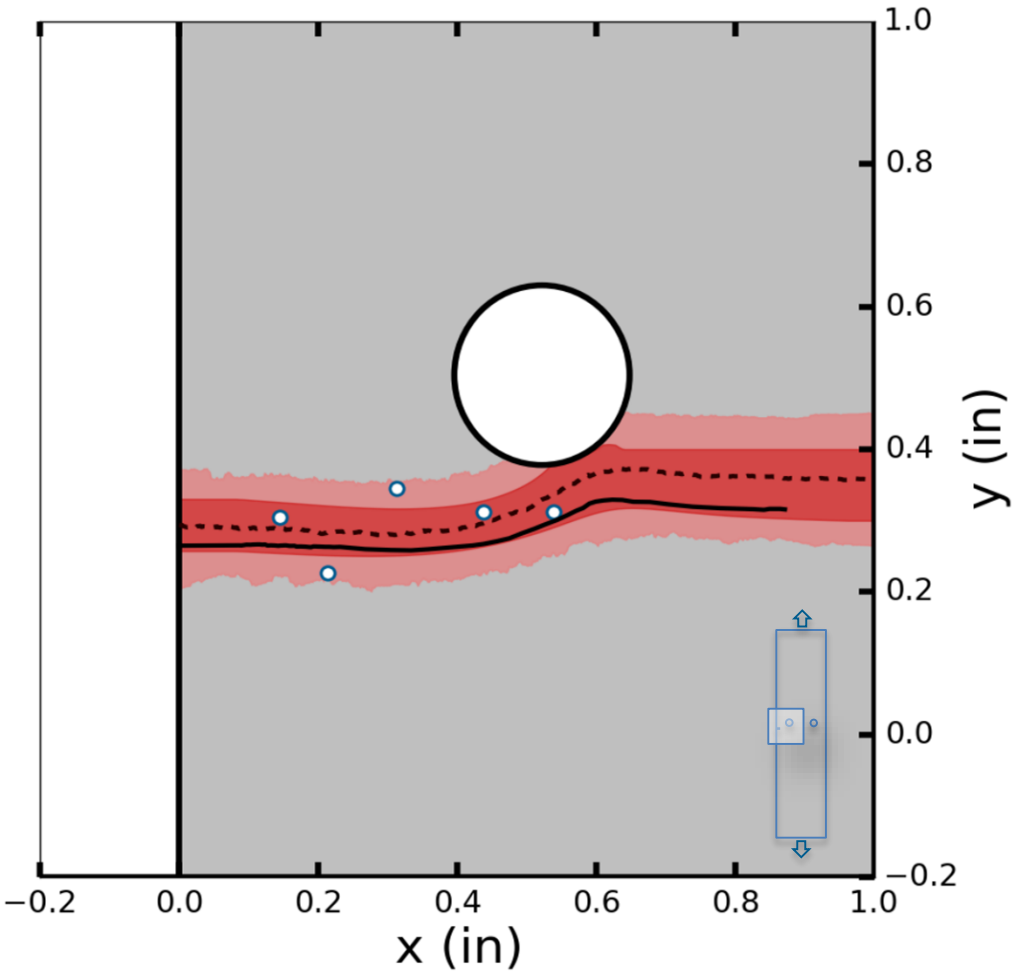
- t_s reduced from 3 hours to 12 seconds
- Markov Chain Monte Carlo (MCMC) using the Python module PyMC [1,2]
- Burn-in: 5,000 samples
- Retained: 10,000 samples
- Thinned: every 10th sample
- Assumed to be unbiased, independently and identically distributed (*iid*) errors
- Random variables:
  - n – the exponential parameter in Walker's modified Paris' Law
  - y_{loc} – the starting location of the crack
- Priors:
  - $n \sim U(0.01, 0.365)$
  - $y_{loc} \sim U(1.0, 6.0)$



1. The Python module PyMC is documented in: Patil, A., D. Huard, and C. J. Fonnesbeck. 2010. "PyMC: Bayesian stochastic modelling in Python," *Journal of statistical software*, 35(4):1-81.
2. The PyMC MCMC sampler is based on the Metropolis-Hastings algorithm found in: Gelman, A., J.B. Carlin, H.S. Stern, and D.B. Rubin. 2004. *Bayesian Data Analysis: Second Edition*. Chapman and Hall/CRC, Boca Raton, FL.

Experimental Validation

Results

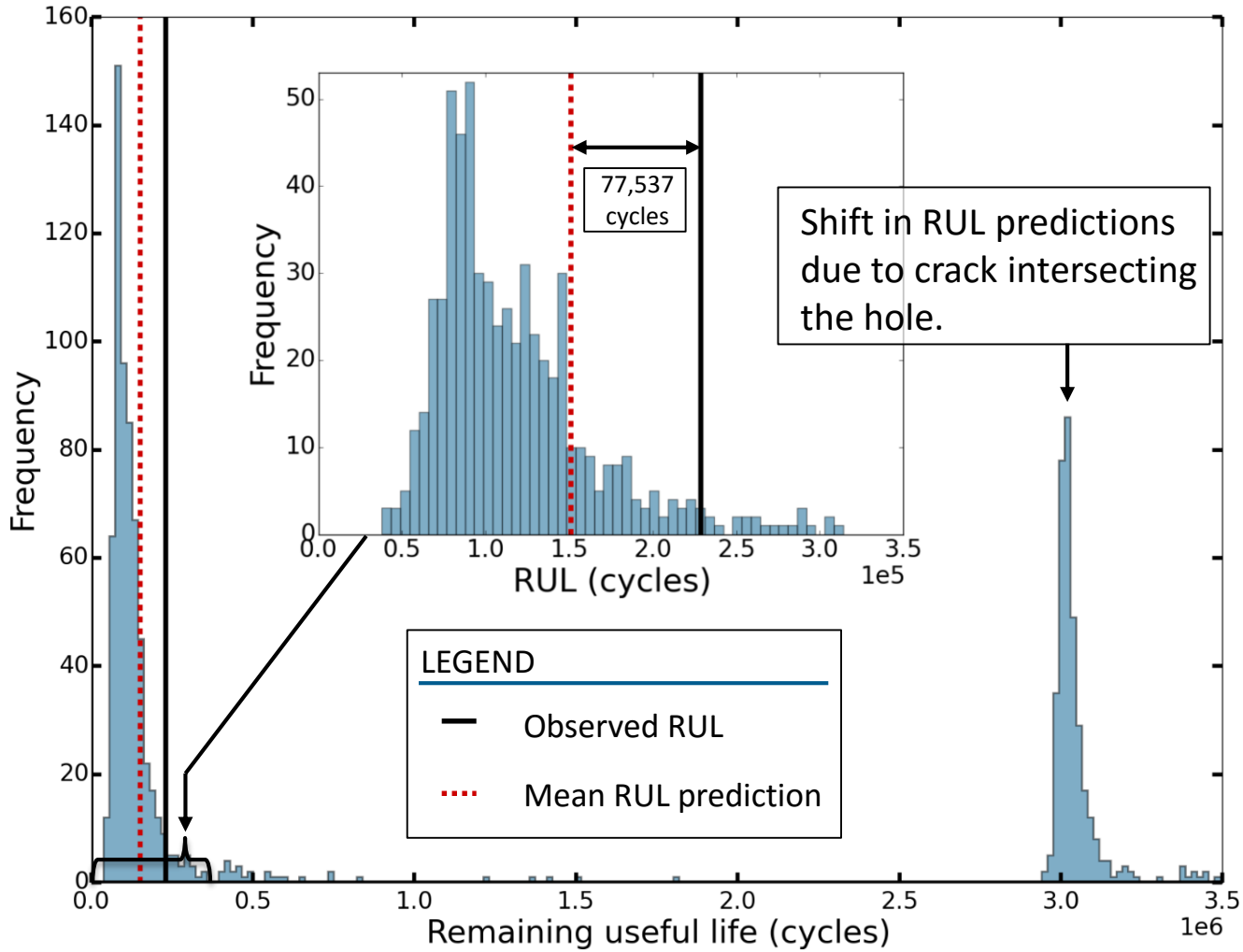


LEGEND

- Observed crack path
- Mean predicted path
- 95% prediction interval
- 95% credible interval
- Visual data (noise added)

Experimental Validation

Results



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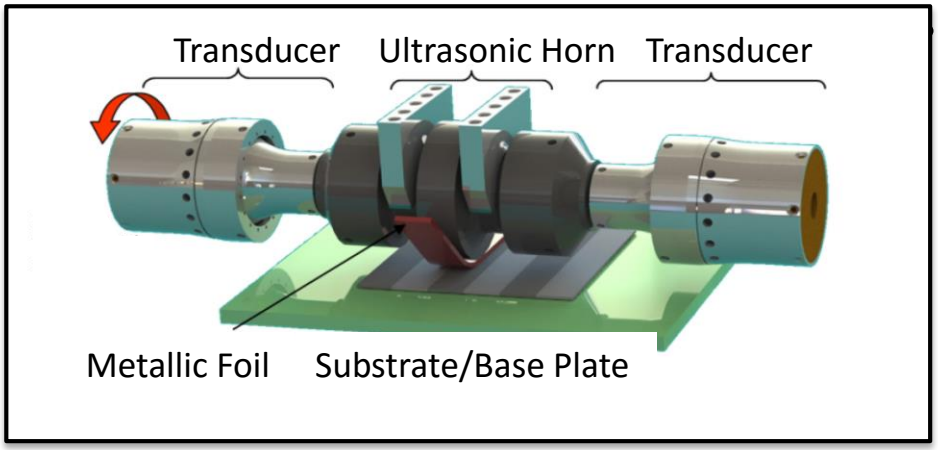
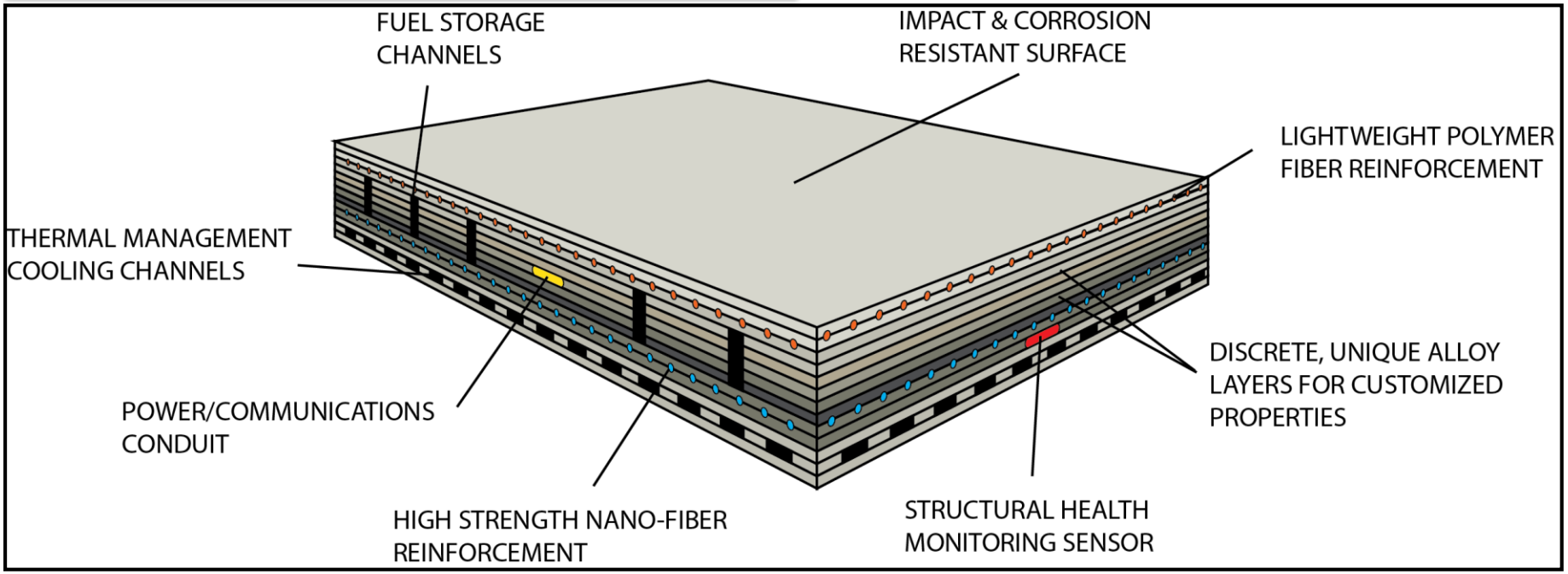
Ultrasonic Additive Manufacturing (UAM)

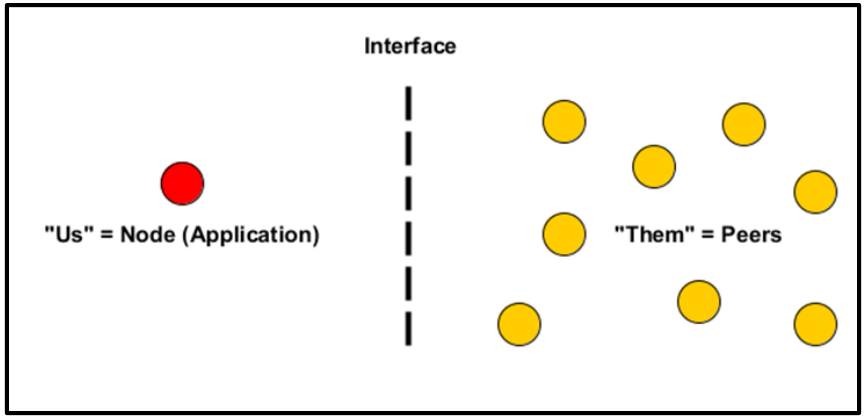


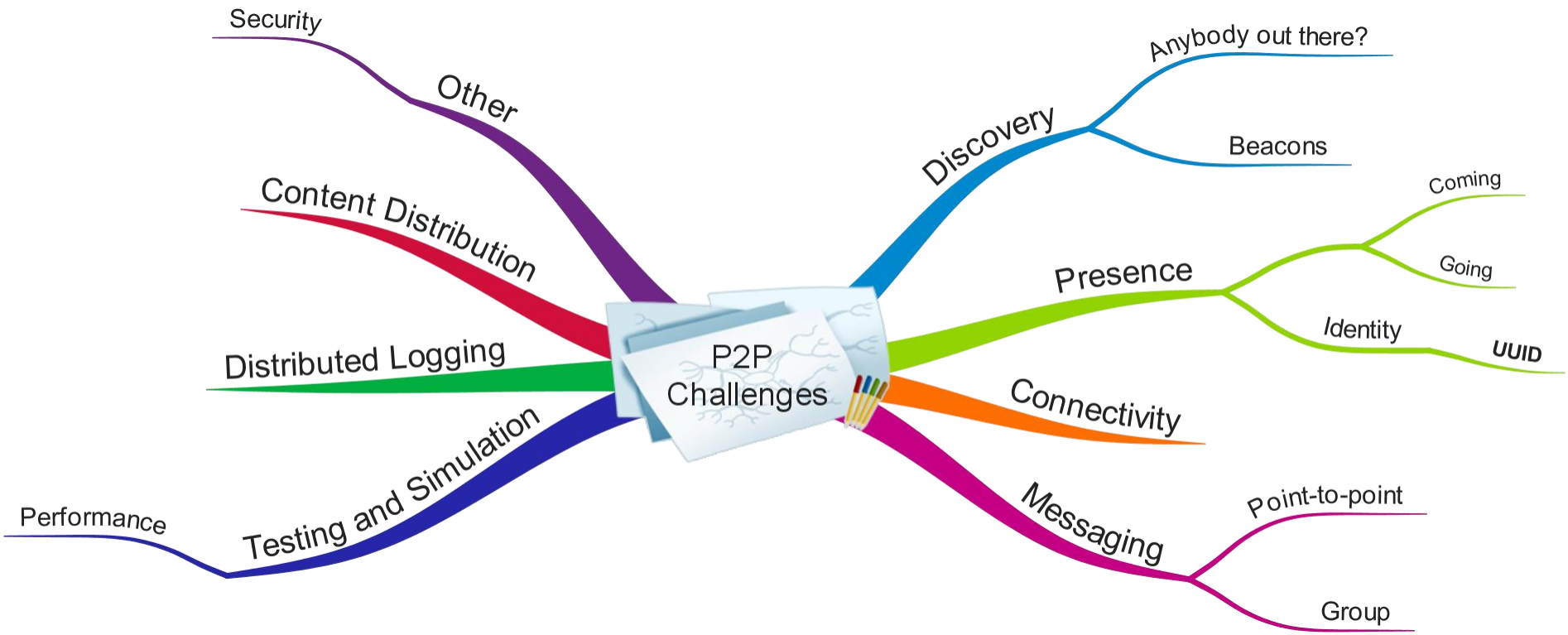
Metallic composite materials produced by ultrasonic consolidation of metal foils

- **Permits configurations not possible by traditional means**

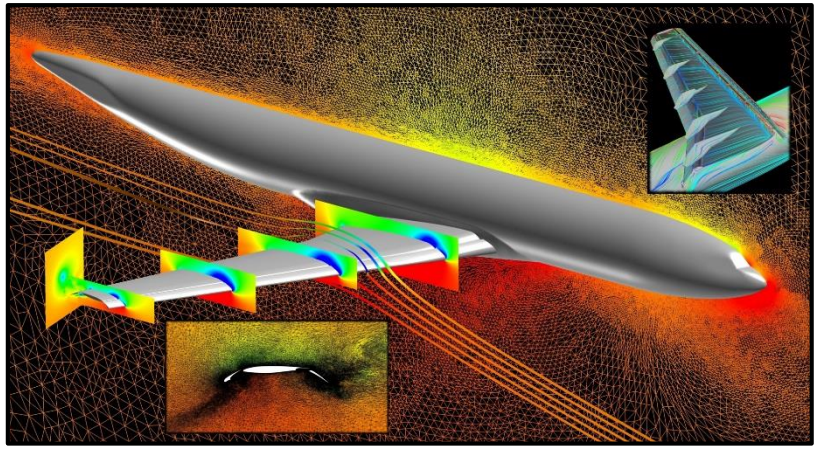


Internet of Simulation Software



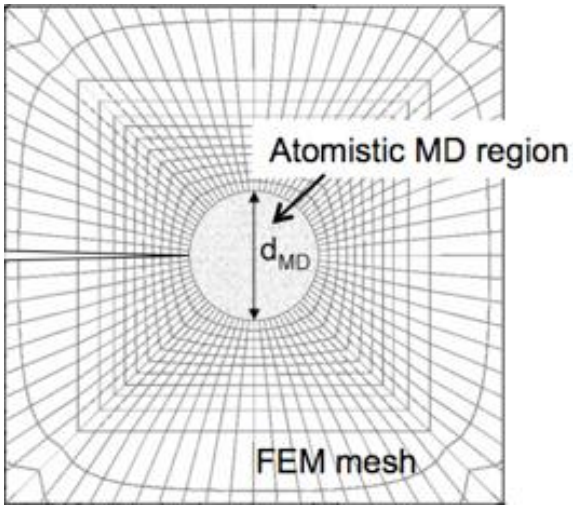


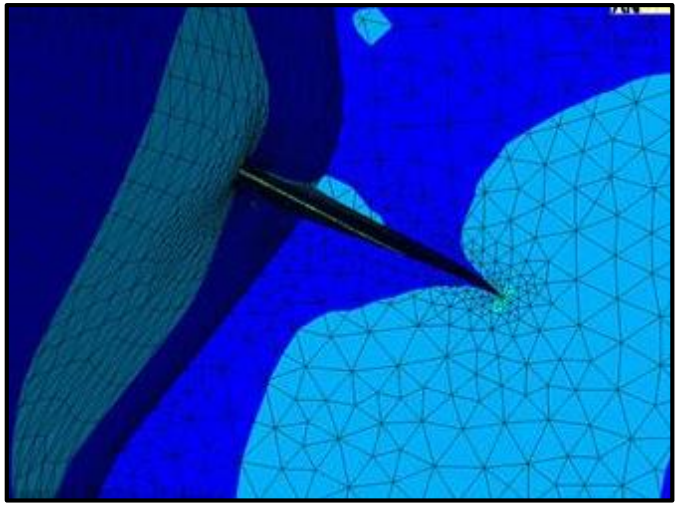
Coupling Simulation Codes



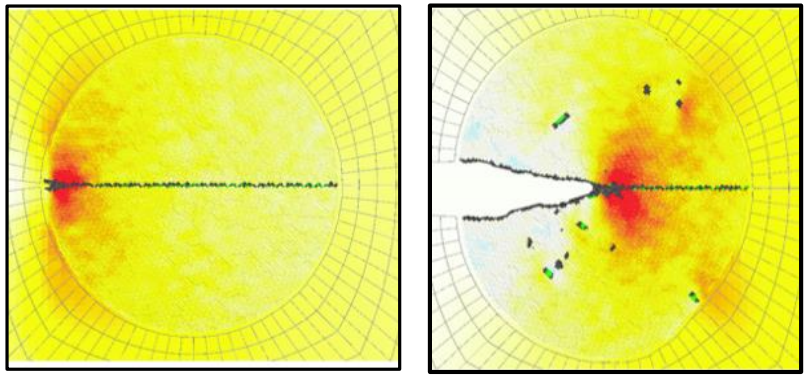
Fluid-structure interaction (FUN3D-ScIFEN)

Coupled MD-FEM
Multiscale Simulations





Fracture Mechanics (FRANC3D)



Summary

- Digital twin = structural health monitoring + personalized modeling and simulation.
  - Proactive (not reactive) maintenance
- Reducing uncertainty via digital twin aims to focus maintenance schedules, alleviate over-design, and speed certification.
- Sensory particles can be used to emit acoustic (or even magnetic) signatures to indicate damage initiation.
  - Ni-Ti particles provided a relatively easy and cost-effective method for obtaining an enhanced acoustic signal.
  - Ni-Mn-Co-Sn particles were investigated to include the ability to detect magnetic changes. However, the material has proven too brittle to function in tensile loading scenarios.
- Reduced order modeling for probabilistic fatigue prognosis was completed and showed orders-of-magnitude speed up in prognosis, while maintaining the fidelity of the more intensive 3D models.
- Digital twin has shown much promise thus far and is continuing as a CAS project during FY16-17.

Selected Patents & Publications

1) J. Hochhalter, A. Cannon, M. Maguire, (2015) "An Efficient Stamping Method for Repeatable Image Correlation Patterning," New Technology Report LAR-18577-1. *Patent application filed. Joint ownership agreement executed with 1900 Engineering LLC (tech. transfer).*
2) P. Leser, J. Hochhalter, J. Newman, W. Leser, J. Warner, P. Wawrzynek, F. Yuan, "Probabilistic Fatigue Damage Prognosis using a Surrogate Model Trained via 3D Finite Element Analysis." In Proceedings of the 10th International Workshop on Structural Health Monitoring, v. 2 (2015) pp. 2407-2414.
3) B. Bielefeldt, J. Hochhalter, W. Leser, D. Hartl, (2015) "Multiscale image correlation for simultaneous strain measurement of particles and near-grip boundary conditions." Invited to submit to special issue of SMS. (*In preparation*)
4) V. Yamakov, J. Hochhalter, W. Leser, J. Warner, J. Warner, T. Wallace, S. Smith, G.P. Purja Pun, Y. Mishin (2015). Multiscale modeling of sensory properties of Co–Ni–Al shape memory particles embedded in an Al metal matrix. *Journal of Materials Science*, 1-13.
5) T.A. Wallace, V. Yamakov, J.D. Hochhalter, W.P. Leser, J.E. Warner, J. A. Newman, G.P. Pun, Y. Mishin, "Computational Modeling and Experimental Characterization of Martensitic Transformations in NiCoAl for Self-Sensing Materials," Proceedings of the 3rd World Congress on Integrated Computational Materials Engineering, Colorado Springs, CO, 2015.
6) W.P. Leser, J.A. Newman, J.D. Hochhalter, V.K. Gupta, F.G. Yuan, "Embedded Ni-Ti Particles for the Detection of Fatigue Crack Growth in AA7050," Fatigue and Fracture of Engineering Materials and Structures. J. Warner, J. Hochhalter (2015) "Propagation of uncertainty and quantification in crack detection from realistic sensor data" Structural Health Management. (*In Review*)
7) J. Hochhalter, W. Leser, J. Newman, E. Glaessgen, V. Gupta, V. Yamakov, S.R. Cornell, S. Willard, G. Heber, (2014) "Coupling damage-sensing particles to the digital twin Concept," NASA/TM-2014-218257
8) A. Cerrone, J. Hochhalter, G. Heber, A. Ingraffea (2014) "The airframe digital twin: a usage case," International Journal of Aerospace Engineering, Volume 2014, Article ID 439278.