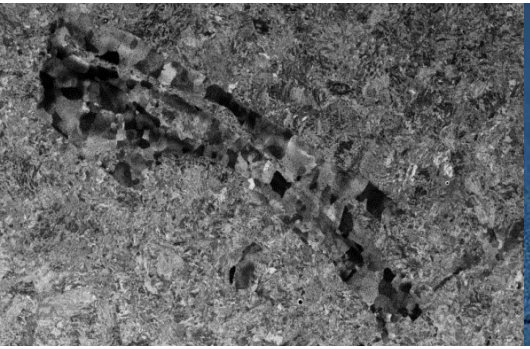
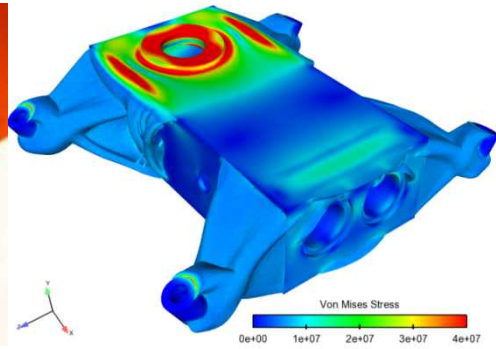
SAND2015-9283C

Exceptional service in the national interest

Sandia National Laboratories



Applications of Material and Computational Science to AM at Sandia

Bradley Jared, PhD

Materials Science & Engineering Center

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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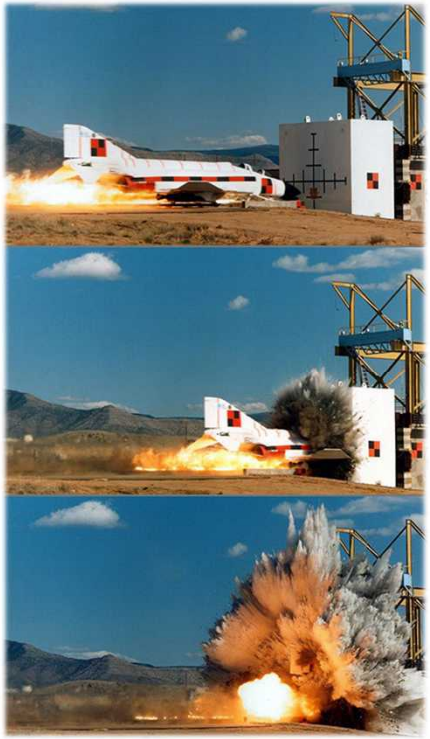
Outline

- Sandia Overview
  - history
  - motivation
  - process capabilities
- Computational Science
  - engineered materials
    - process simulation
    - predicting material performance
  - design optimization
- Material Science
  - material assurance challenges
  - critical defects in metal powder bed fusion (PBF)

Sandia National Laboratories

- A National Security Science & Engineering Laboratory
  - "Exceptional service in the national interest"
- Nuclear Weapons
- Defense Systems & Assessments
- Energy & Climate
- International, Homeland, & Nuclear Security

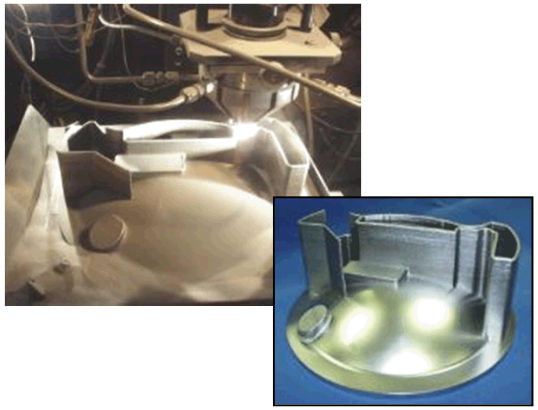


Sandia Has a Long History in AM

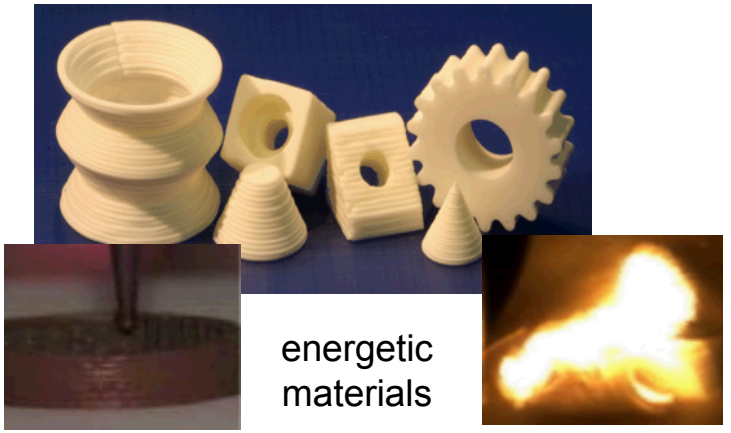
- 30+ yrs of pioneering AM tech development & commercialization

FastCast*
prototype test unit

LENS®*
fireset housing

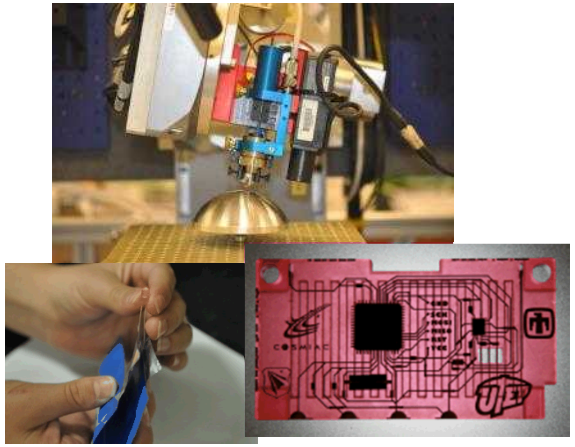


RoboCast*
ceramic parts

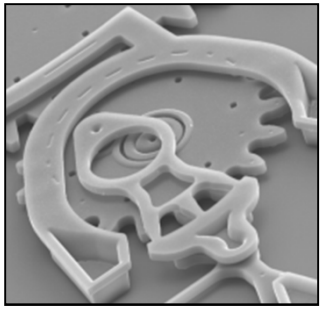


energetic materials

Direct Write
conformal electronics

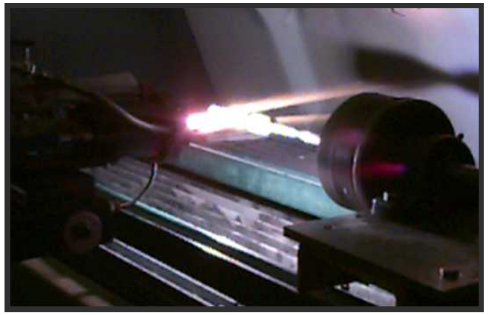


MEMS SUMMIT™*
micro gear assembly



LIGA
"Hurricane" spring

Spray Forming
rocket nozzle



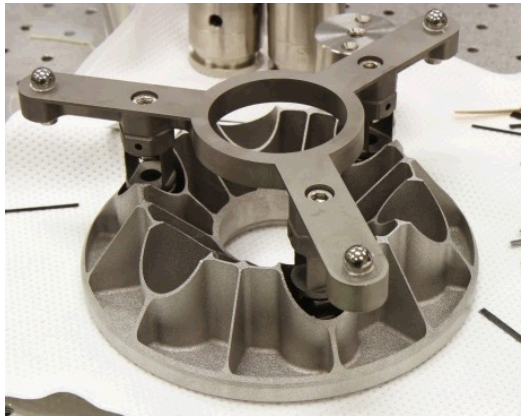
* licensed/commercialized technology

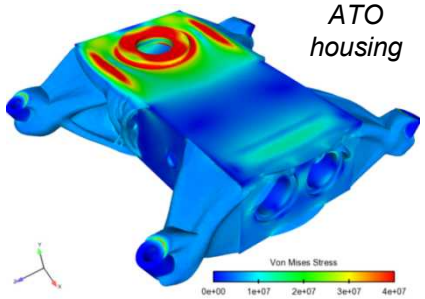
SNL's Additive Interest

- Reduce risk, accelerate development
  - simplify assembly & processing
  - prototypes, test hardware, tooling & fixturing
    - > 75-100 plastic machines
    - cost reductions often 2-10x
- Add value
  - design & optimize for performance, not mfg
    - complex freeforms, internal structures, integration
  - engineered materials
    - gradient compositions
    - microstructure optimization & control
    - multi-material integration

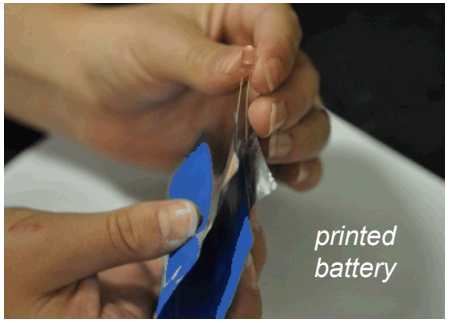
Sandia Hand, 50% built w/AM, cost ~$10k

prototype Al AM mirror & structure

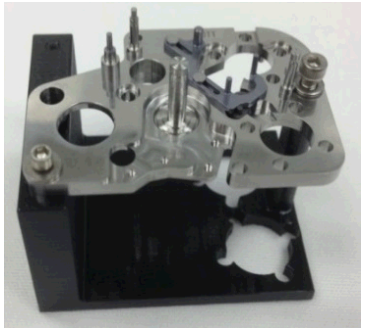




ATO housing



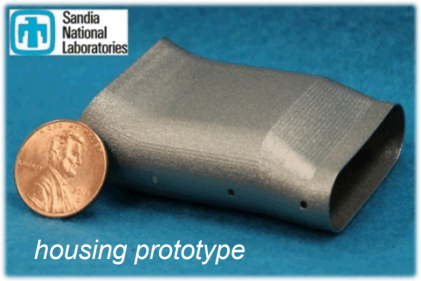
printed battery

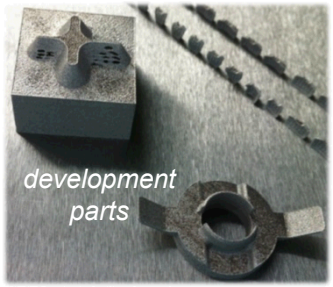


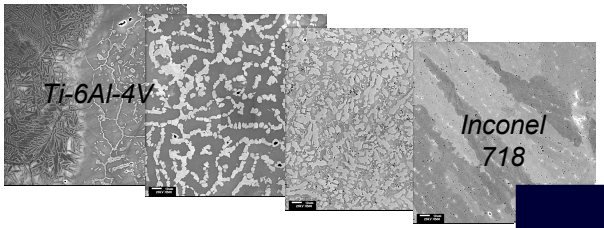
fixture generated in 1 day

Metal Additive

Powder bed

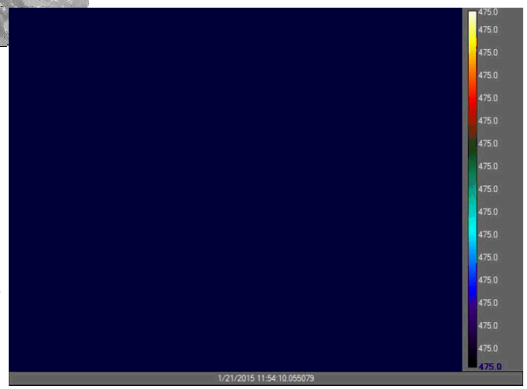




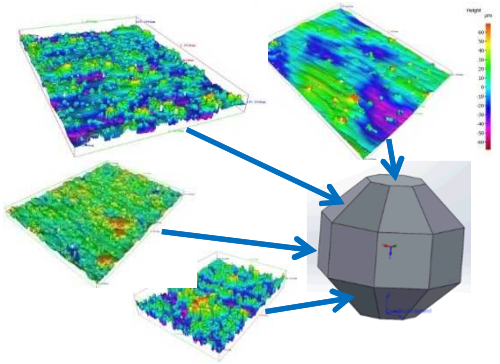


functionally graded materials

LENS



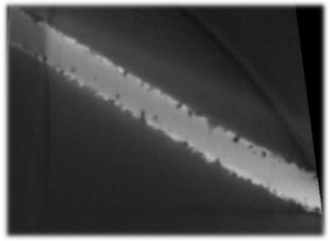
thermal history during bi-directional metal deposition



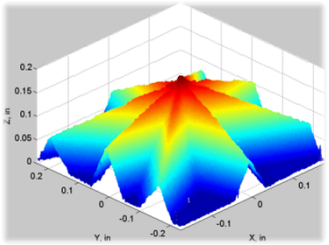
17-4PH polyhedron texture anisotropy map

Metrology

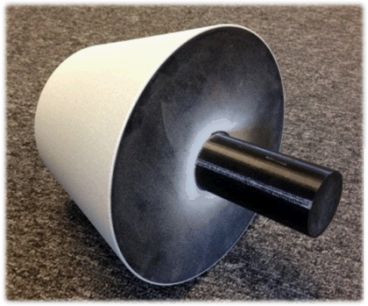
"Death" star for process evaluation



17-4PH voids & defects w/CT

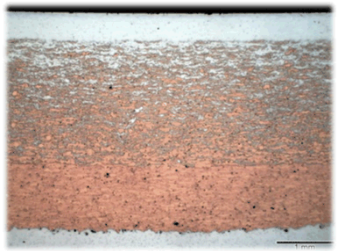


Ti6Al4V Siemens star data



3D printed mandrel w/thermal sprayed zinc

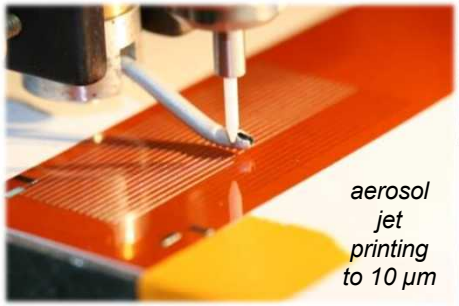
Thermal spray

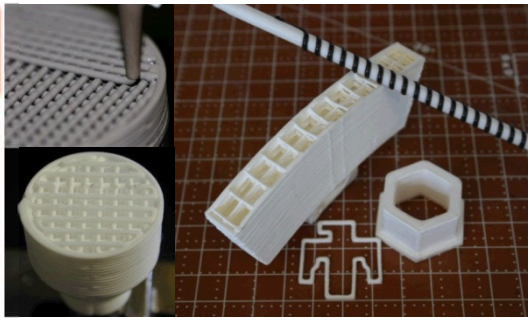


Cu-Al plasma sprayed graded density coating

Bradley Jared, Dan Kammler, Larry Carrillo, David Keicher, John Smugeresky, Josh Sugar, Aaron Hall, Pylin Sarobol, Hy Tran

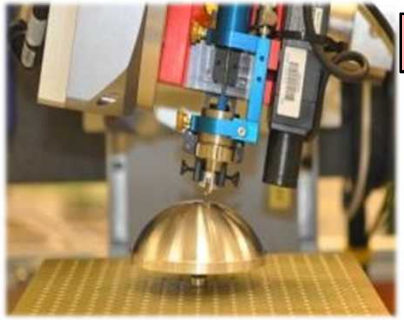
Direct Write



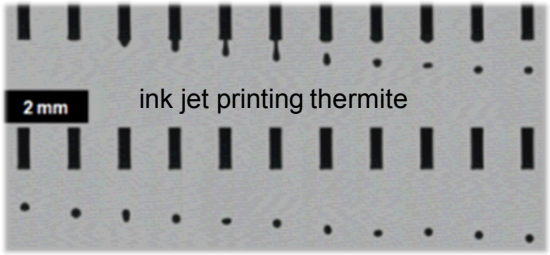


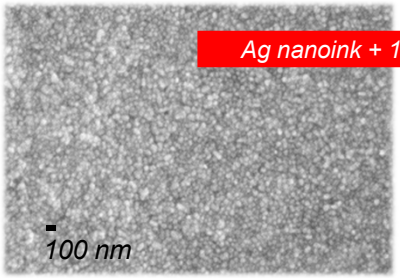
extrusion casting (Robocasting)

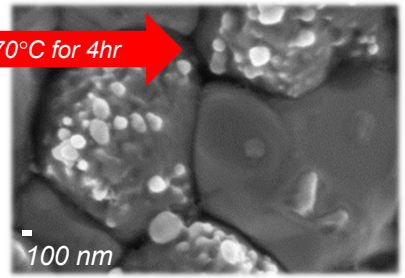
Process



conformal printing

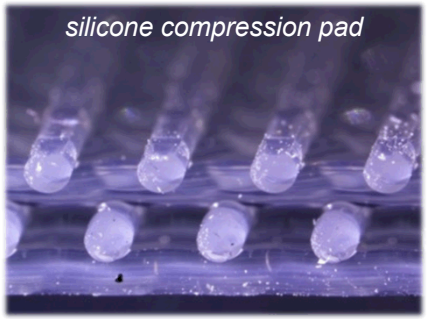


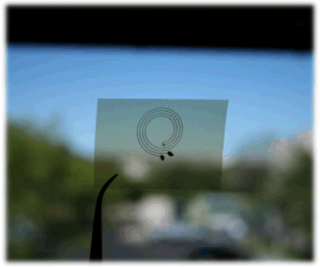




sintering of Ag nanoinks for conductive pathways

Materials

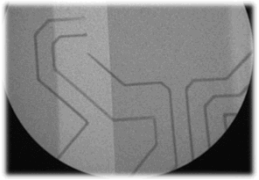




room temperature cure
of Ag traces on PET film

Ag traces on
powdercoated metal

circuit fabrication

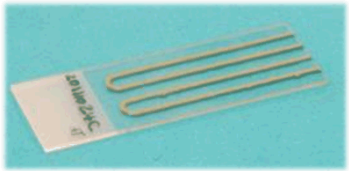


X-ray of 4 layer
composite

rapid circuit prototyping & production
for thick film LTCC

printed battery

energetic materials

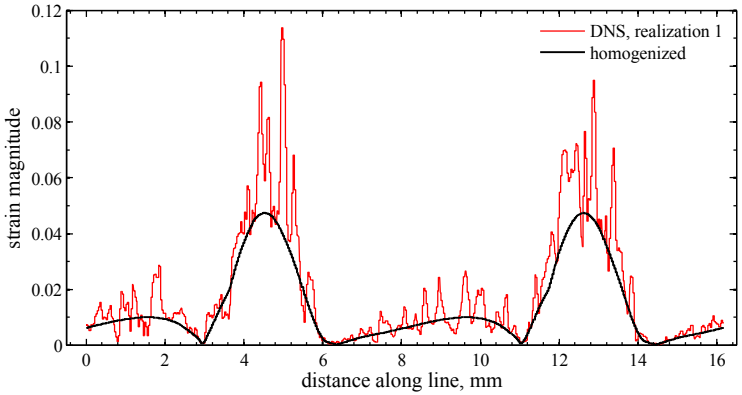


Applications

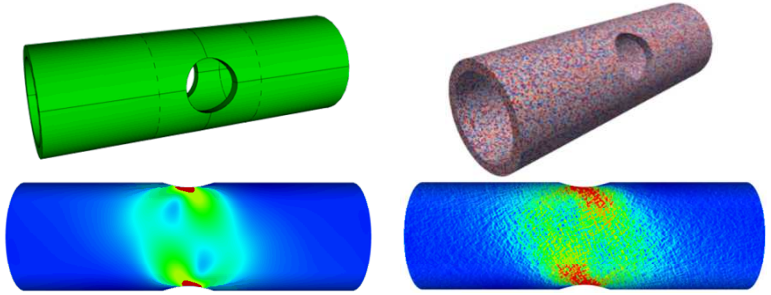
Adam Cook, David Keicher, Alex Tappan, James Hochrein, Robert Bernstein

Engineered Materials

- Integrated Computational Materials Engineering (ICME)
  - materials analog to mechanical engineering
  - microstructure matters
- Voxel access introduces new opportunities for control & design
  - spanning multi-scales is difficult
  - metallurgical limits exist

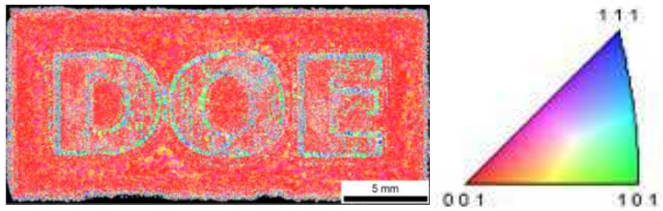


strain field due to tension-torsion

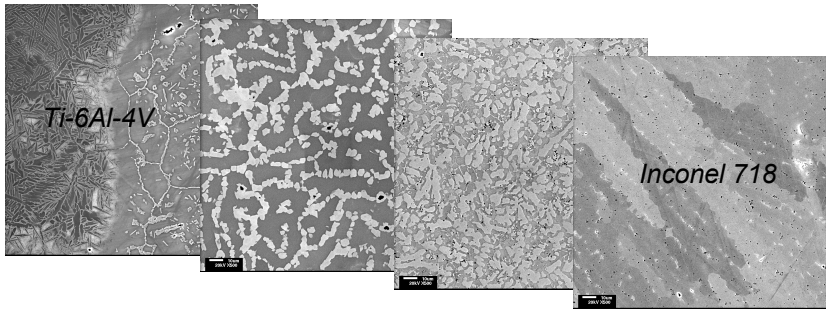


continuum model *crystal plasticity model*

AM Inconel 718 texture control demo by ORNL

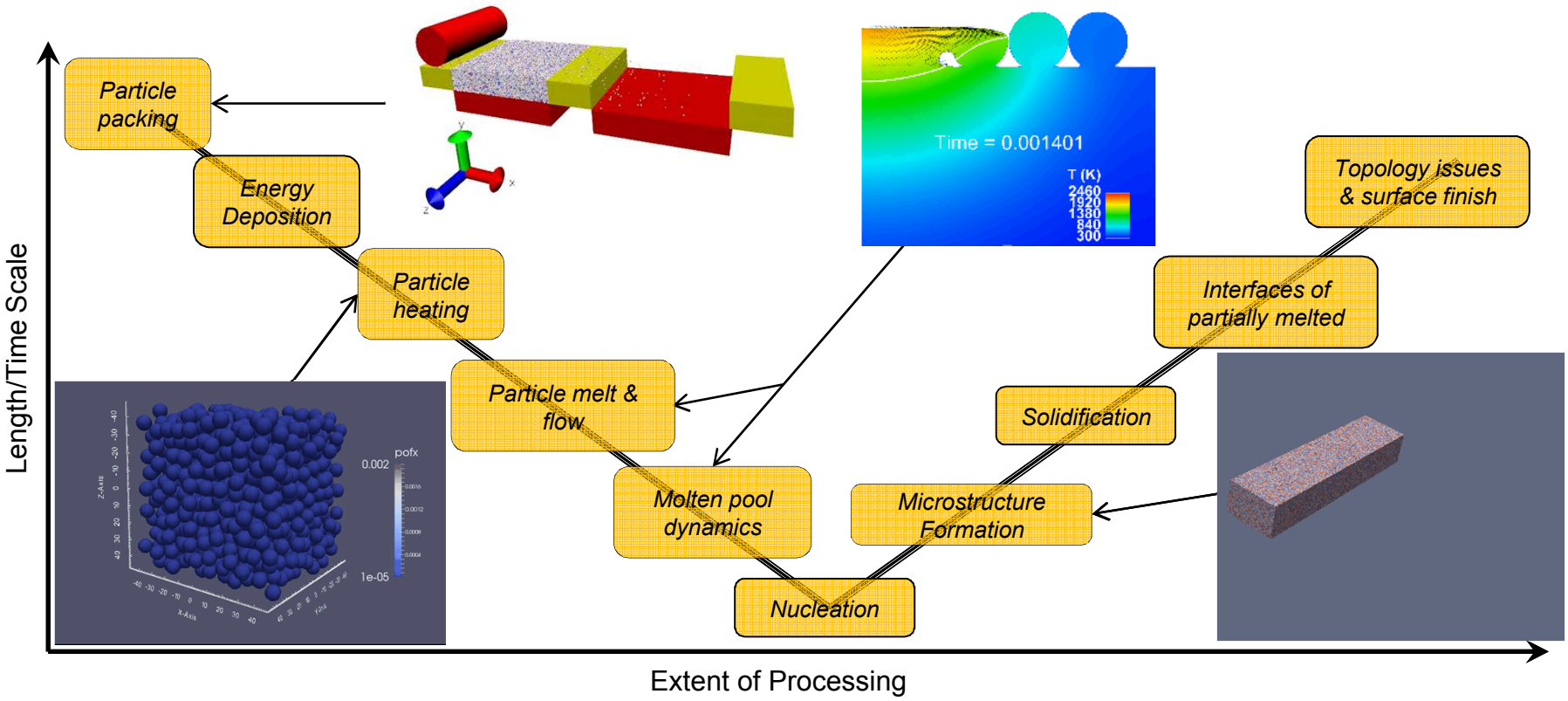


"We can now control local material properties, which will change the future of how we engineer metallic components," R. Dehoff



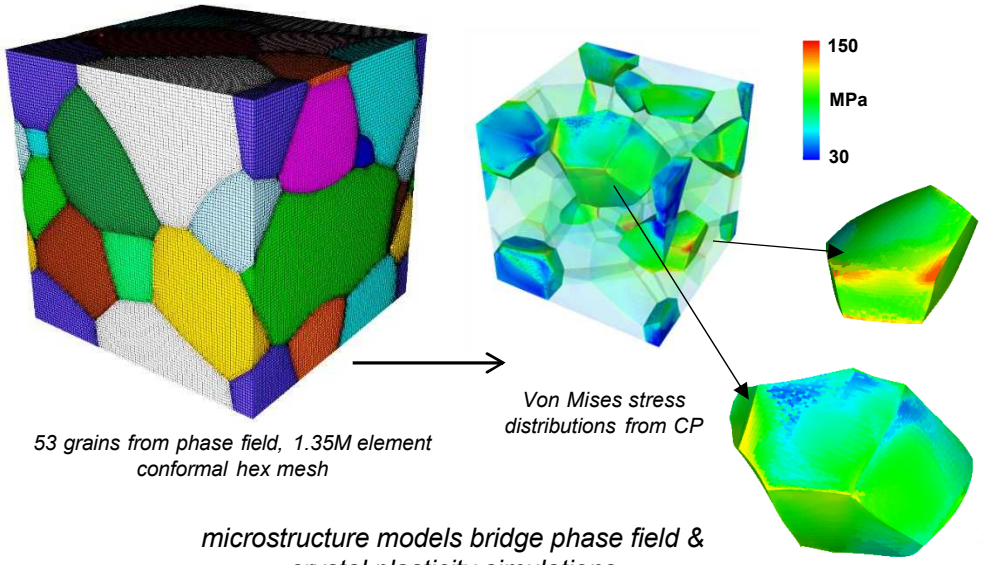
LENS® functionally graded materials

Application of Process Simulations



- Process
  - reduce experimentation
    - laser-material interaction
    - discrete particle physics
  - process -> structure relationships
  - process limits
- Defect impact
  - understand formation mechanisms
  - explore uncertainty quantifications
  - predict response from stochastic process knowledge

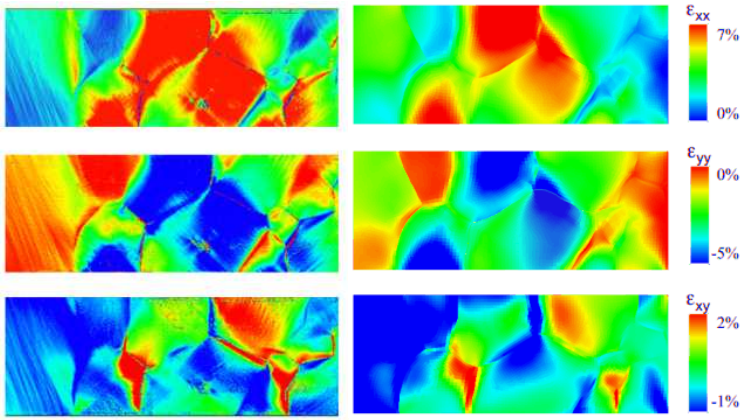
Predicting Material Performance



53 grains from phase field, 1.35M element conformal hex mesh

Von Mises stress distributions from CP

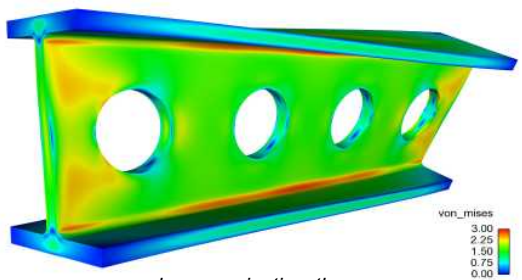
microstructure models bridge phase field & crystal plasticity simulations



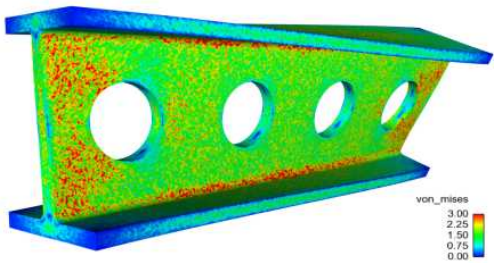
DIC measurements

simulations

oligocrystal tensile load experiment vs. crystal plasticity models

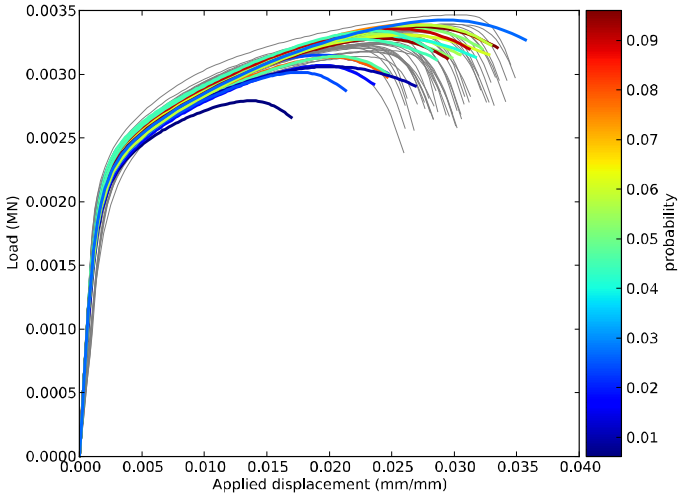


homogenization theory



Direct Numerical Simulation (DNS)

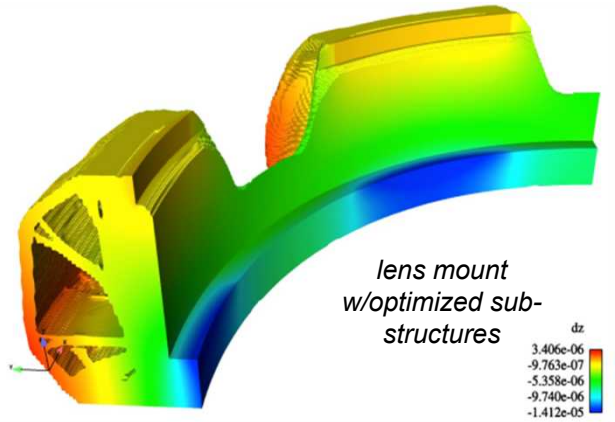
macroscale torsion stress fields



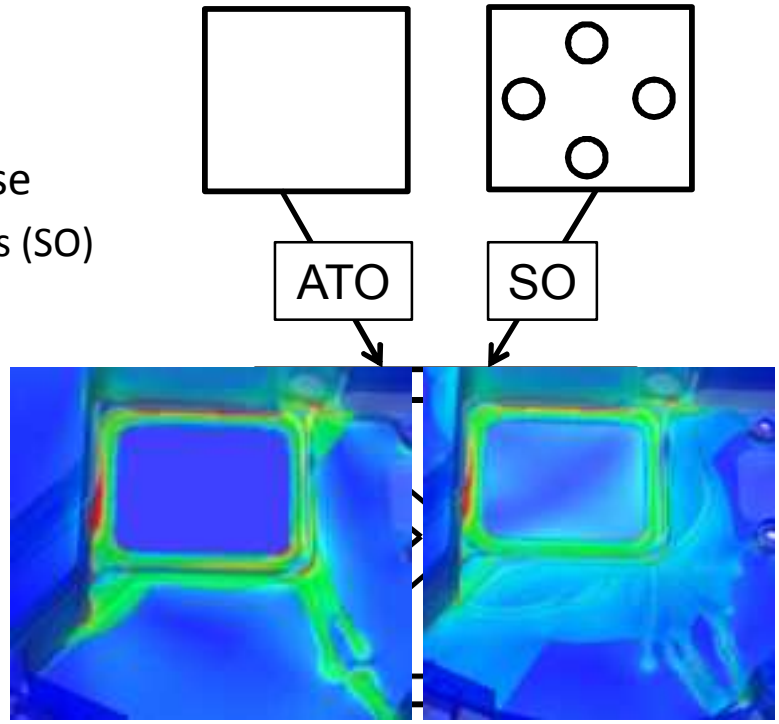
predicted (color) vs. measured (grey) response for welds (PPM)

New Design Freedom

- Computational synthesis for optimal material use
  - adaptive topological (ATO) & shape optimizations (SO)
  - leverages “complexity is preferred”
  - constrained by performance requirements
  - bio-mimicry requires AM
  - design occurs concurrent w/simulation



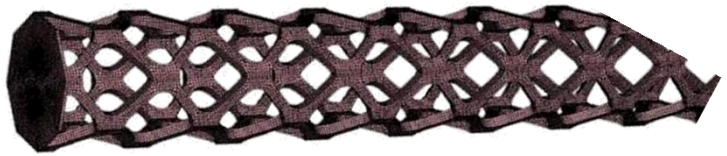
lens mount w/optimized sub-structures



+ 0.55% volume
- 52% deflection

+ 3.3% volume
- 64% deflection

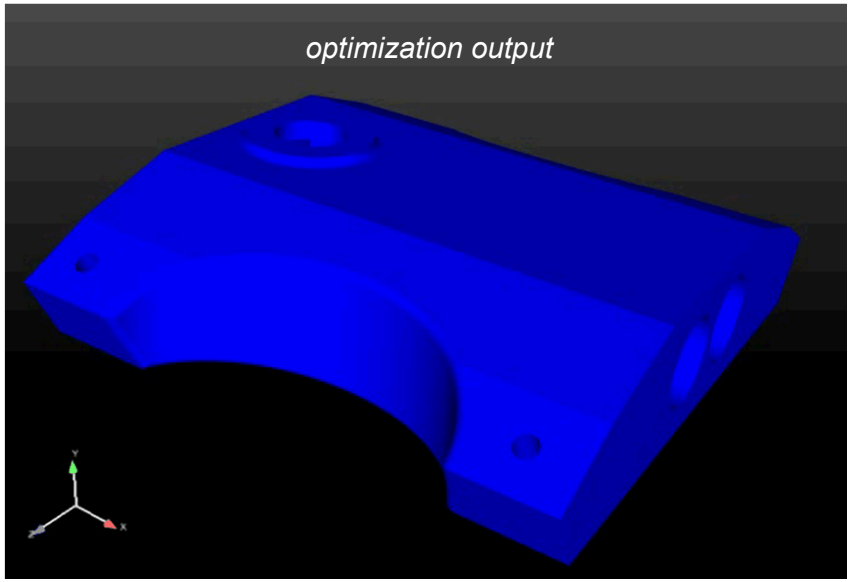
elasto-static stiffness optimization

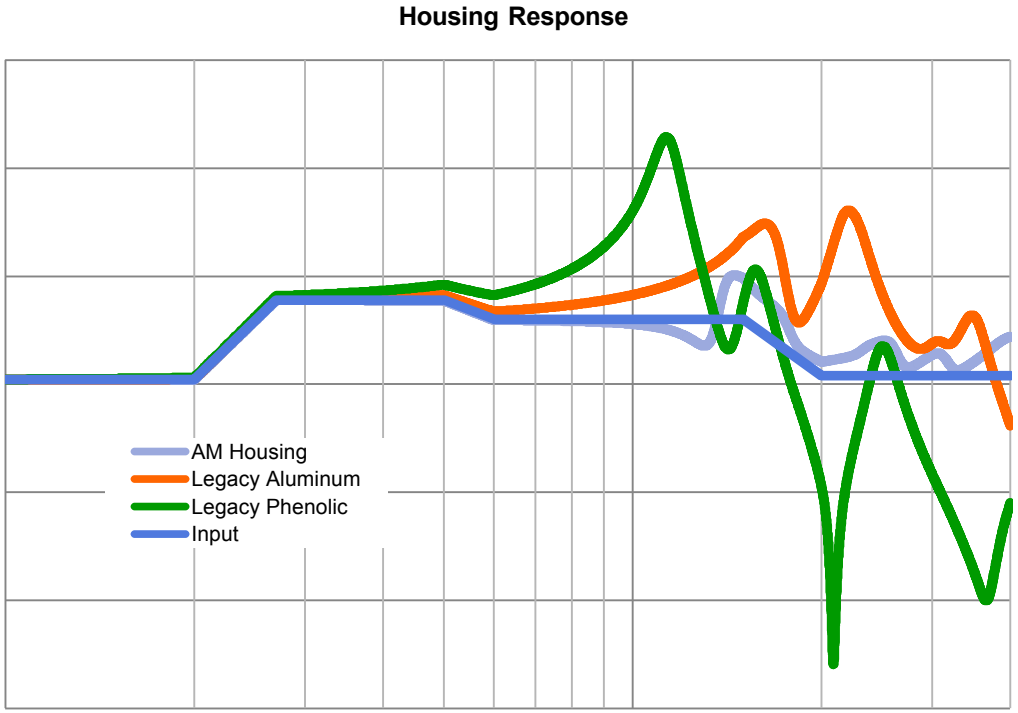


solution for a bar in pure torsion resembles a cholla cactus

Optimization Impact

Optimized design (using same mass and material, i.e., carbon phenolic) achieves 39% average increase in modes of interest, compared to 23% increase achieved by printing original design in aluminum.



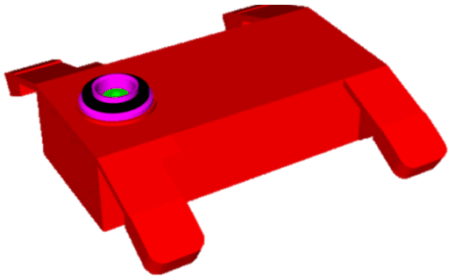


Inverting the Design Cycle

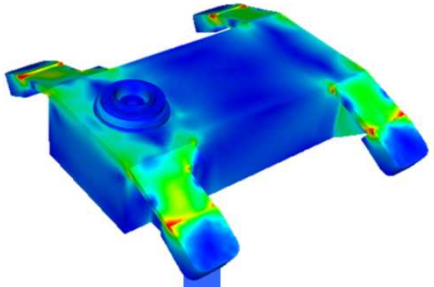
CURRENT

Specify Form

Design



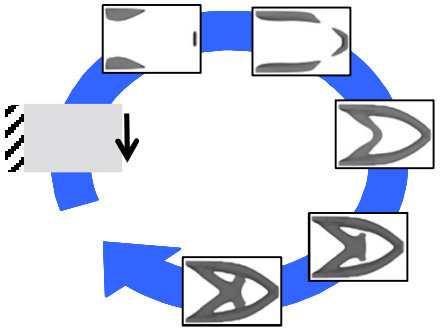
Verify Function Using FEA



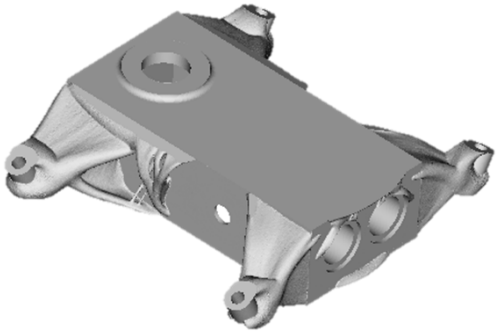
NEW

Specify Design Domain and Function

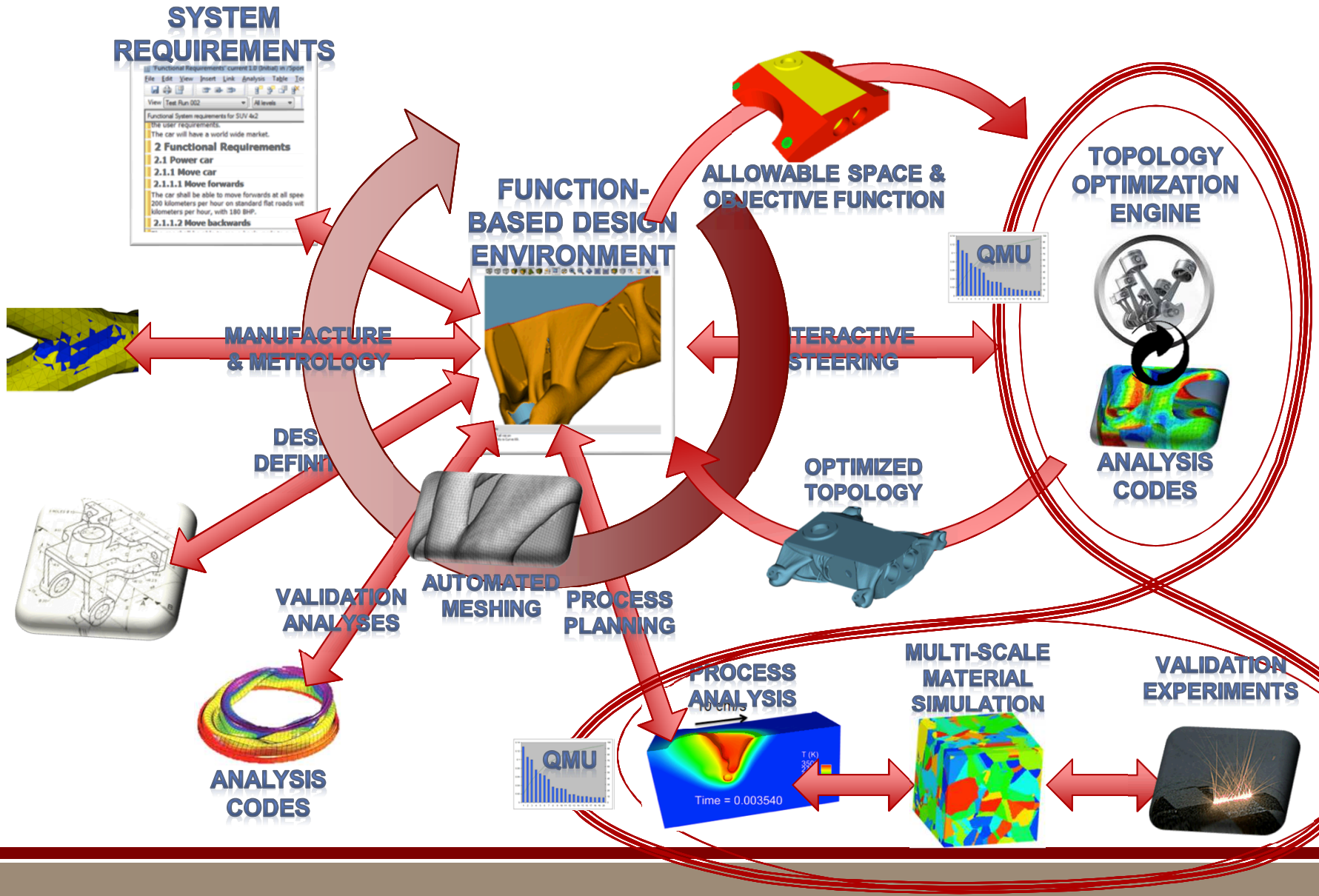
Use Topology Optimization (FEA) to Determine Form that Meets Function



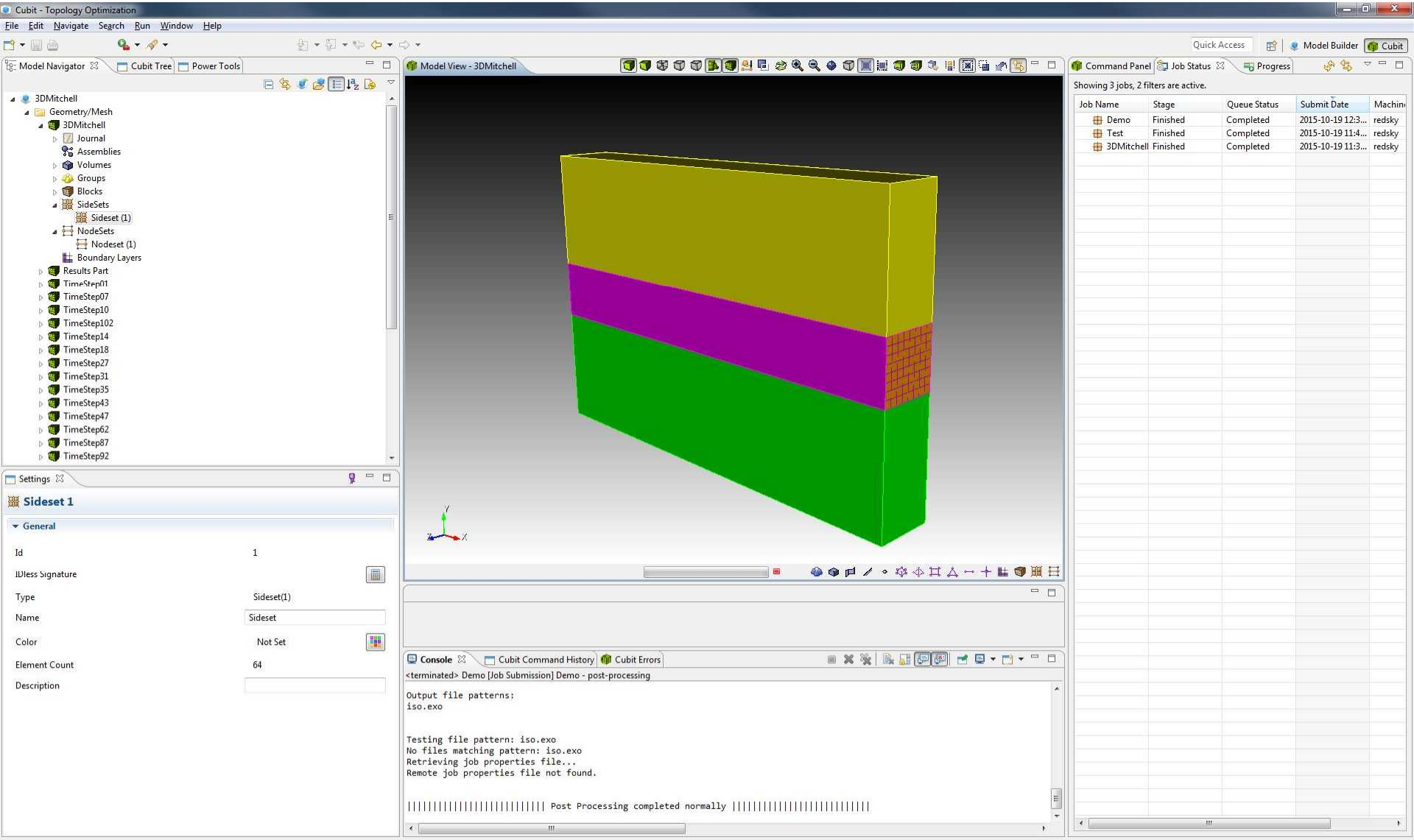
Optimized Design (Form)



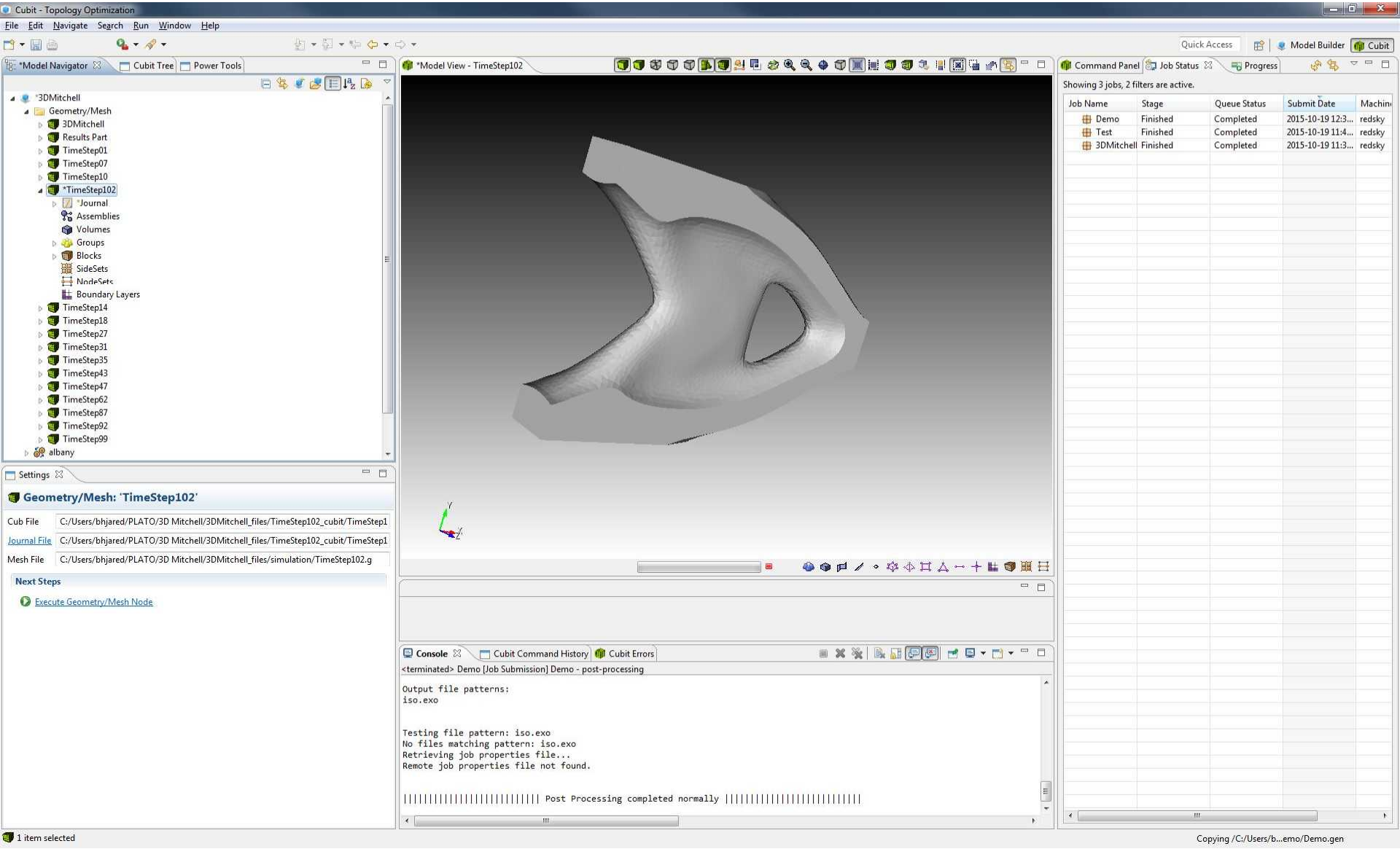
How Will This Revolution Work?



Sandia Analysis Workbench (SAW)

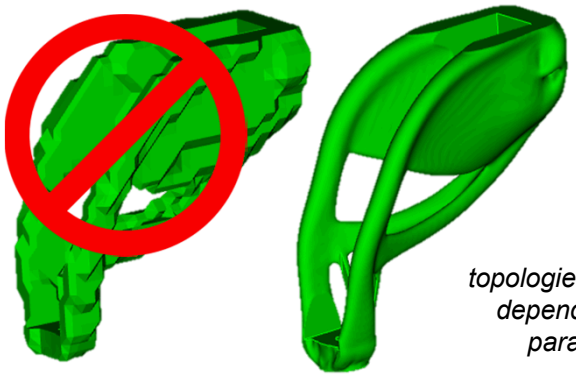


Sandia Analysis Workbench (SAW)

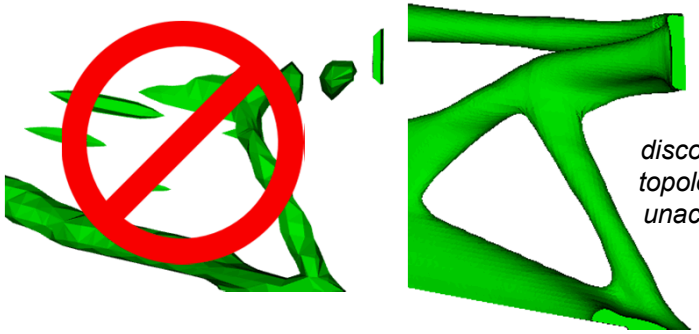


Design Challenges

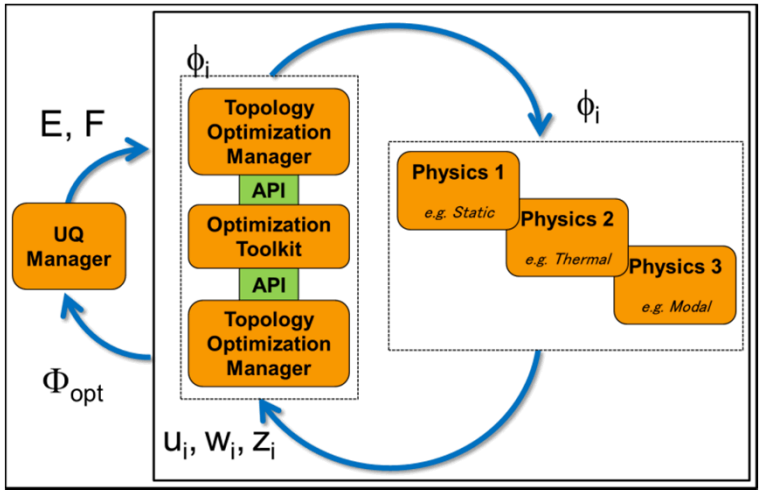
- Ease of use
  - data formats
  - interactive steering
  - smooth, connected geometries
- Efficiency
  - manipulating volume data
  - reduced order models
  - faster converging algorithms
- Physics
  - elasto-statics, modal, thermal exist
  - complex boundary constraints (ex. sliding)
  - multi-physics
  - process constraints & design rules
- Uncertainties
  - computational, requirements, materials
  - solve stochastic inverse problem



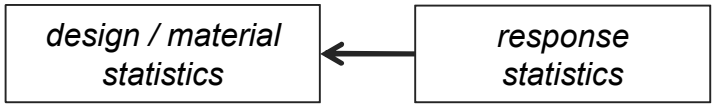
topologies & surfaces depend on mesh parameters



discontinuous topologies are unacceptable

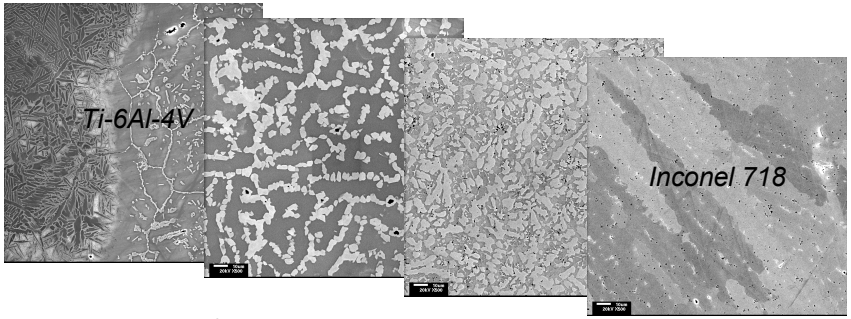


optimization scheme



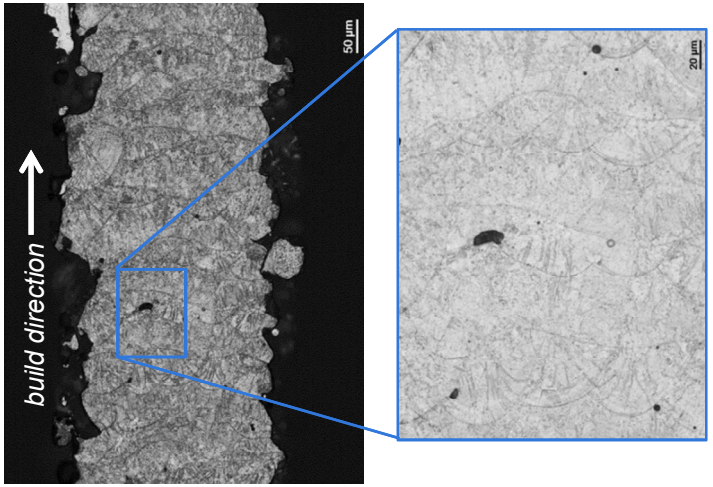
Challenges Managing Additive Metals

- Material formation concurrent w/geometry
  - feedstock certs inadequate for performance
  - how to ID a bad part?
    - ex-situ evaluation can be too slow, expensive, inaccurate &/or late
    - need worst case properties & distributions, not just the mean
  - complexity isn't "free"
    - traditionally just measured surfaces
    - properties vary w/geometry



LENS® functionally graded materials

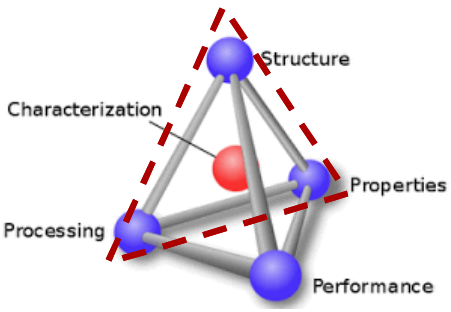
- Processes
  - predominantly open loop
    - enables large margins or post-process inspection
    - unacceptable for high consequence parts
  - process monitoring becoming available
    - defect detection
    - path to moderate margins & yields (?)



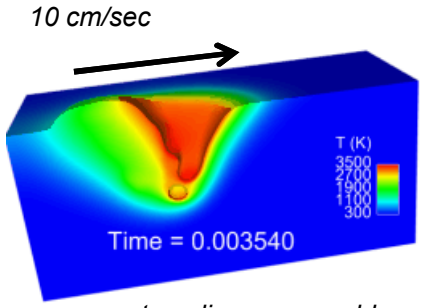
defects in 17-4 PH w/ 0.015" nominal wall thickness

New Paradigm for Material Assurance

- Quantify process-structure-property relationships
  - process maps, constitutive models & HPC simulations
  - *understand behavior & formation of <u>critical</u> defects*

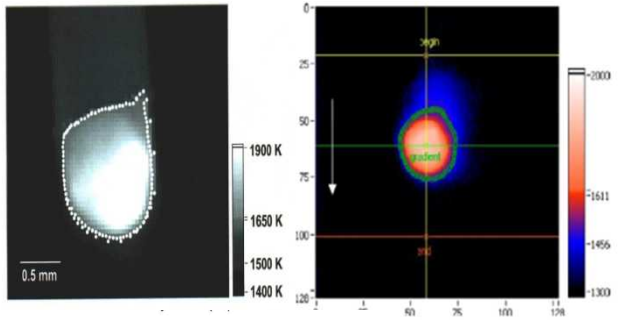


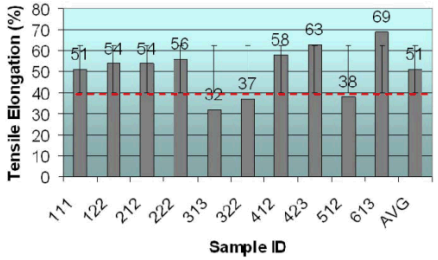
materials tetrahedron



traveling seam weld (Sierra, Martinez)

- Implement process control
  - start w/in-situ monitoring
    - establish property bounds & control needs
  - predictive process control
    - defect prevention (and correction?)
    - material optimization



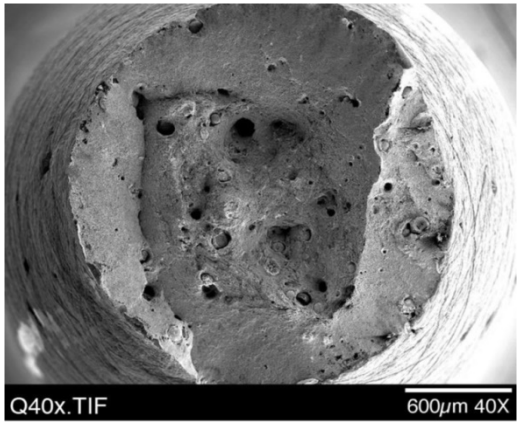


LENS® control of melt pool & microstructure

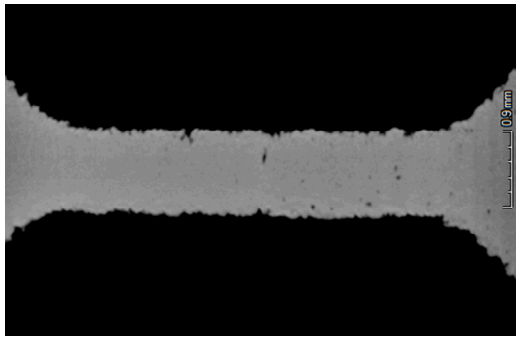
- Leverage experience in LENS®, laser welding , thermal spray, casting

Exploring *Critical* Defects

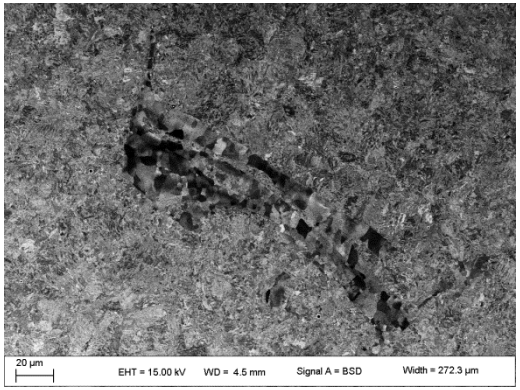
- Characterize, predict & control for metal powder bed fusion
  - exploring PH13-8Mo as an alternative to 304L
    - initial work in 17-4PH
  - higher strength w/multiple strengthening mechanisms
- Quantifying morphologies & distributions
  - micro-CT, destructive sectioning
  - multi-modal analyses
    - grain orientation, composition, localized hardness, micro-segregation, secondary phases
  - what can we ID accurately & efficiently?
- Understand mechanistic impacts on properties
  - characterize stochastics
  - build structure-property relationships



*ductile fracture initiated by LENS® defects in PH13-8Mo**



CT of 17-4PH dogbone sample



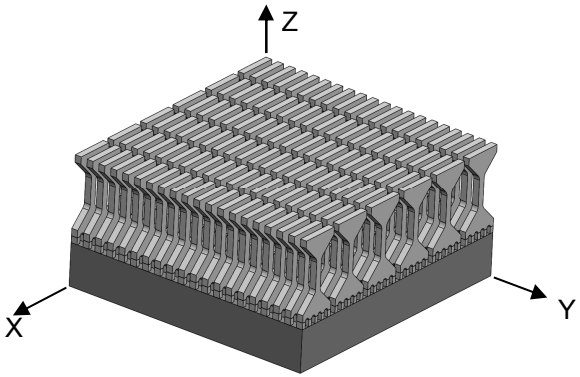
untransformed ausetnite+ferrite in 17-4PH

* *Microstructure and properties of PH13-8Mo steel fabricated by LENS, Zheng, Smugeresky, et al*

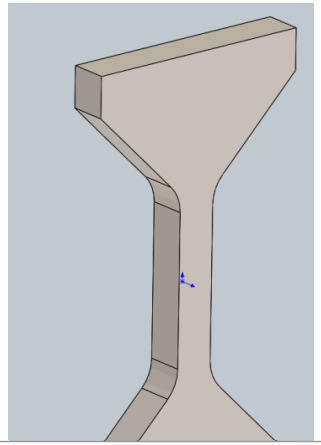
Tensile Testing

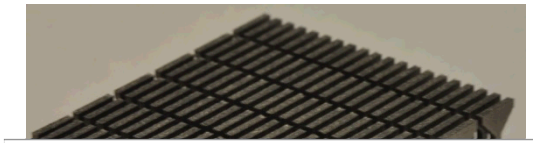
- Characterizing stochastics
  - ***large sample sets***
  - ***high throughput***
    - approaching 100/hr
  - custom dogbone test sample
    - follows ASTM guidelines
  - using digital image correlation (DIC)
    - off-line analysis

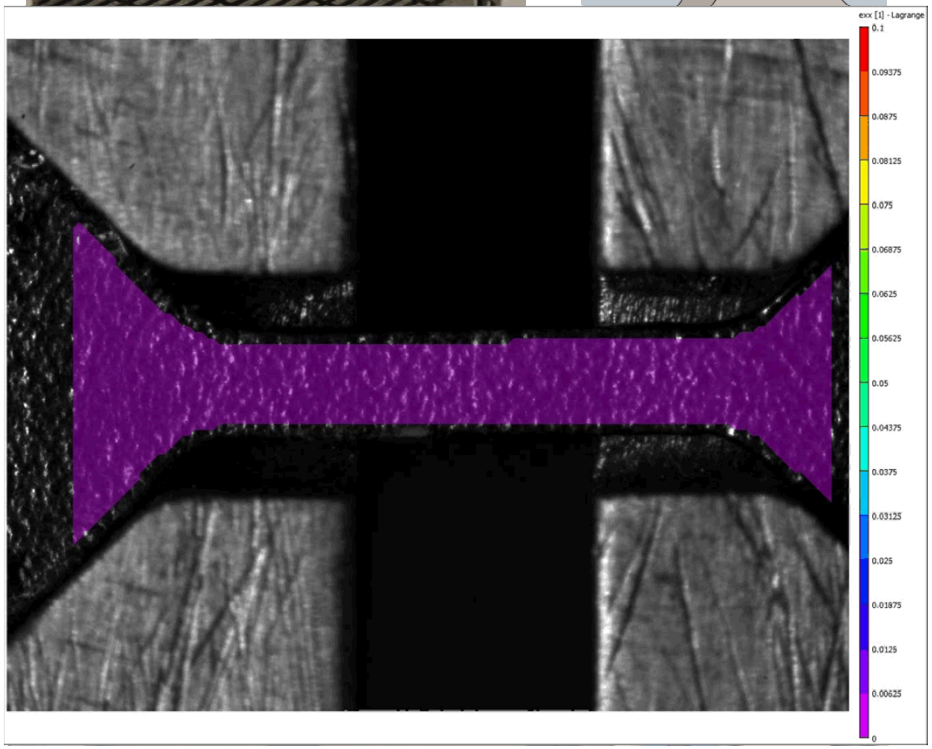
- Initial testing
  - 0.4, 1.0, 2.5 mm square gage sections
  - "constant" build process from two vendors
    - vertical build orientation
    - individual part locations tracked
  - exploring heat treatment, build orientation & process parameters



"cooling fin" dogbone sample

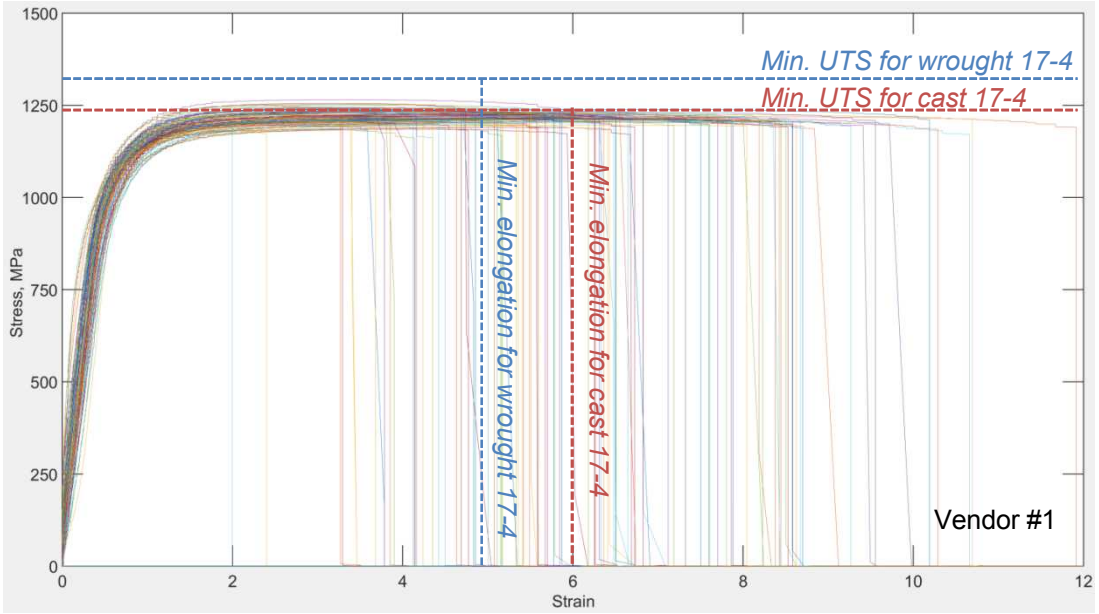


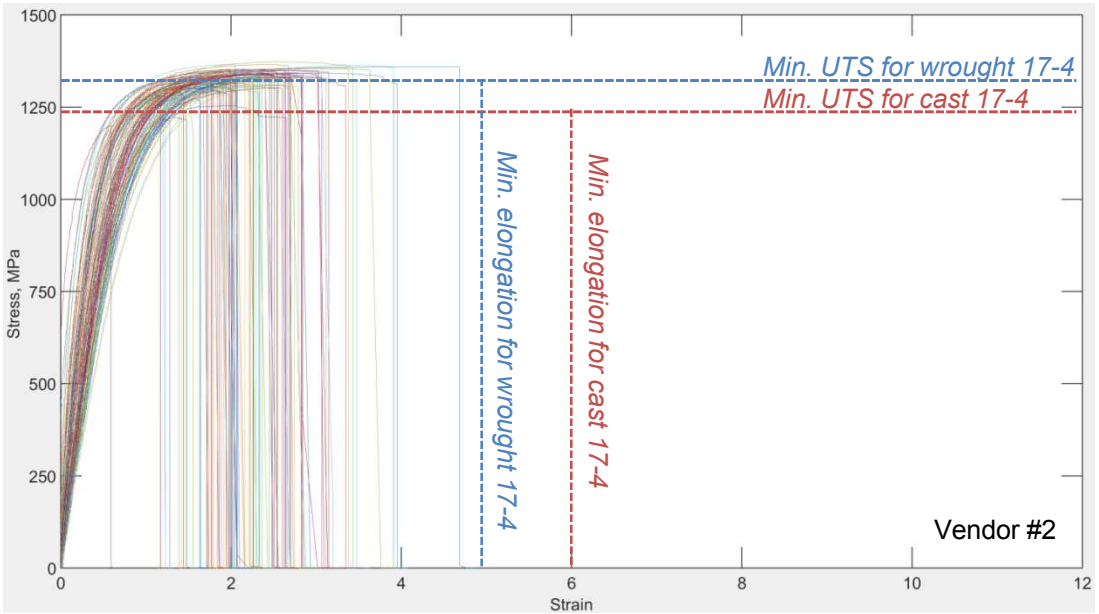




Tensile Data

- Two vendor sets
  - 104 samples each
  - H900 heat treatment
  - Vendor #1
    - bead blasted
  - Vendor #2
    - no bead blasting
- Observations
  - vendor differences
  - strength & ductility variations
  - AM vs. wrought / cast





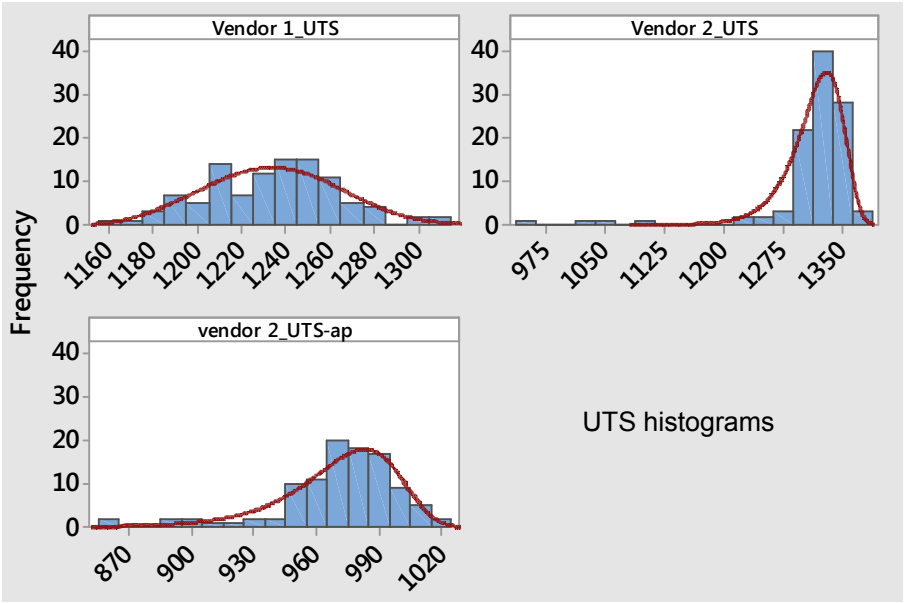
AMS spec for H900: modulus = 197MPa, yield = 1172MPa, UTS = 1310MPa, strain at failure = 5%

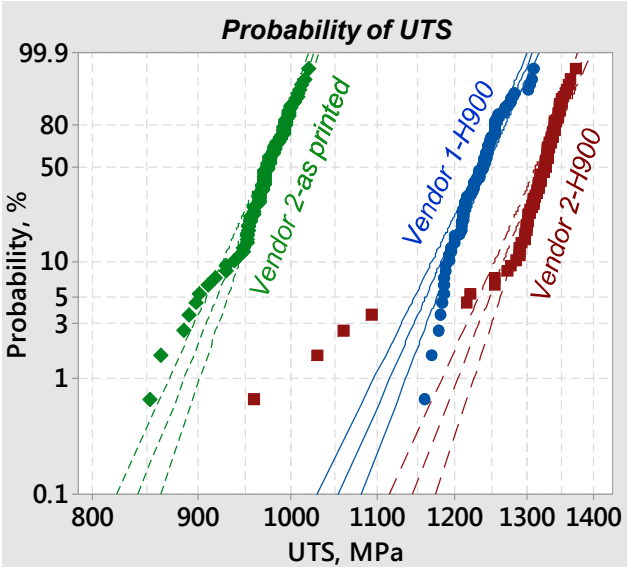
Material Distributions

- Data variation suggests defect dominated failure
  - Similar to ceramics, castings
- Weibull distributions prove appropriate

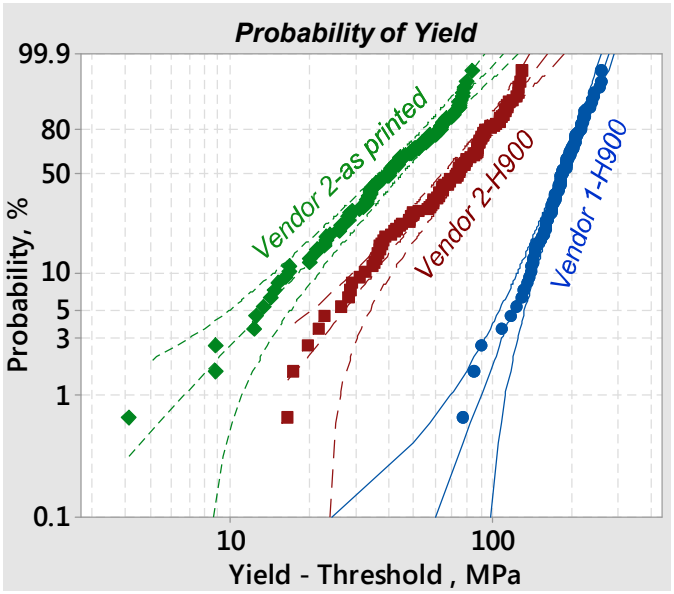
$$log\left(log\left(\frac{1}{1-P}\right)\right) = m \cdot log(\sigma) + log\left(\frac{V \cdot log(e)}{{\sigma_o}^m}\right)$$

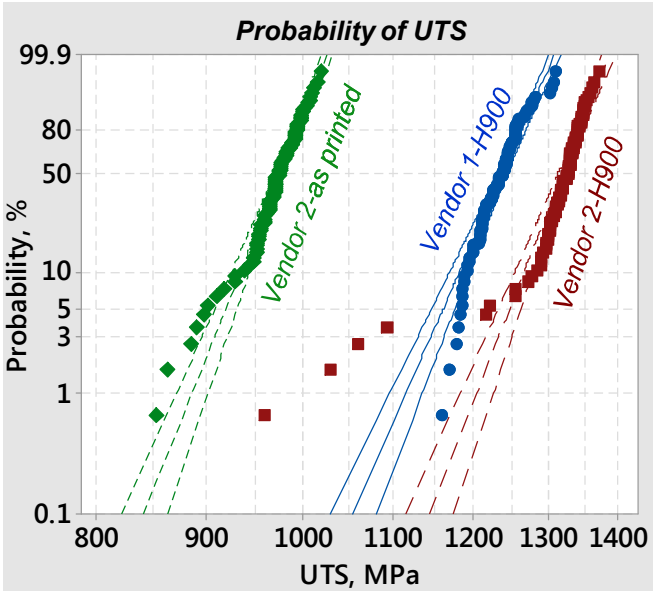
  - where
    - P = probability of failure at stress, σ
    - m = Weibull modulus, i.e. scatter
    - V = material volume
    - σ_o = strength for which $P = 0$

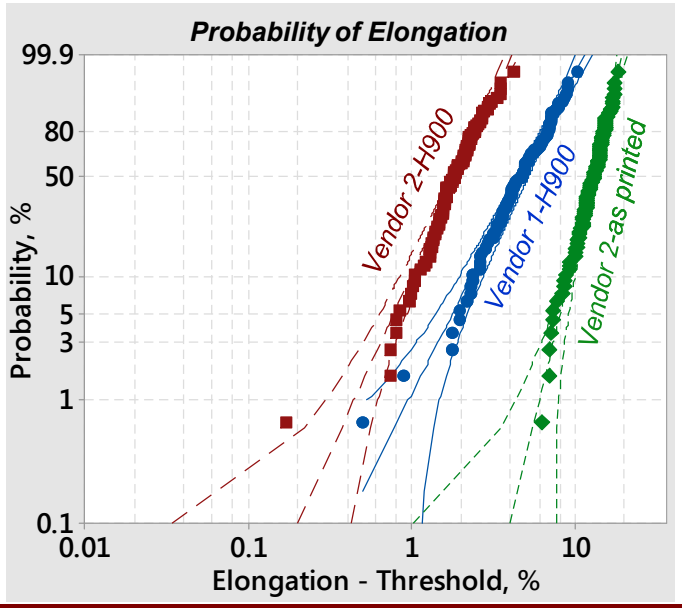


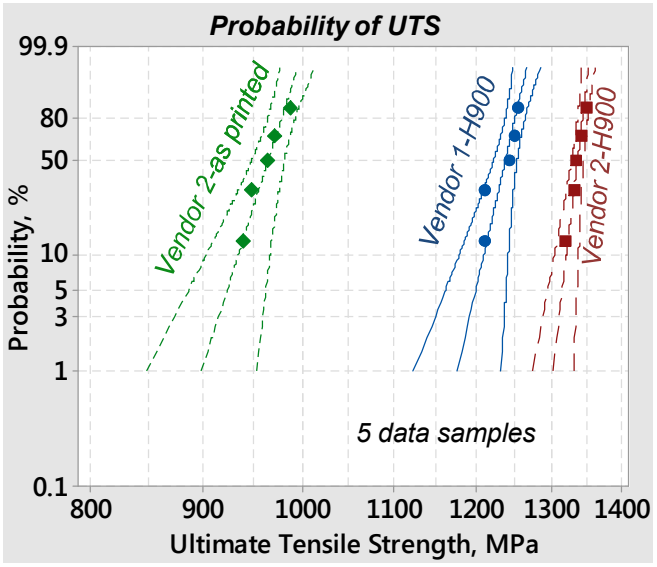


Material Distributions



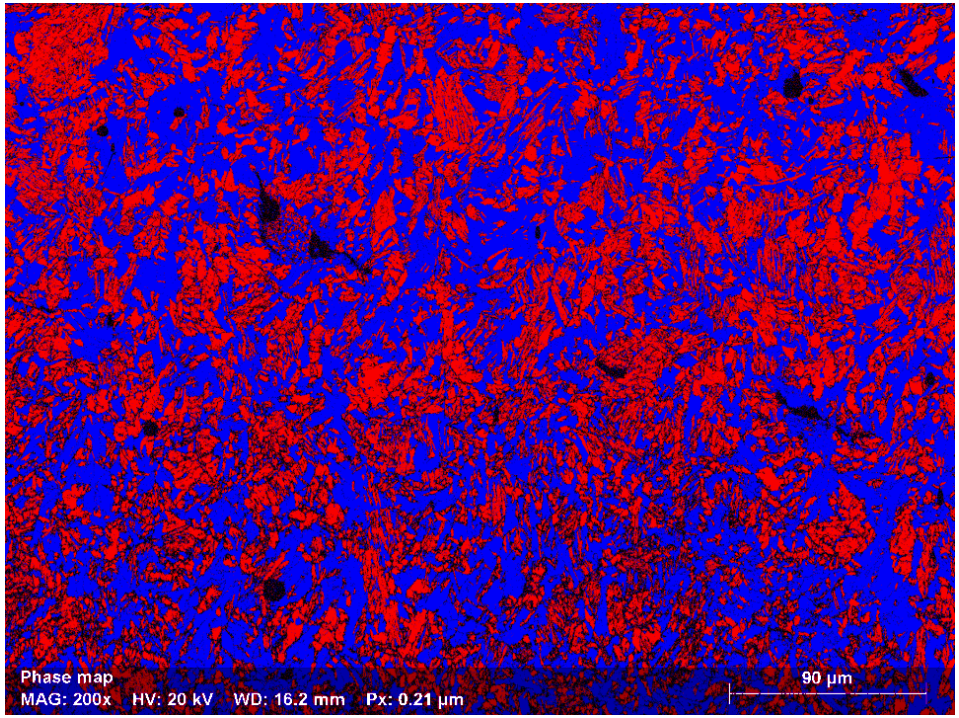




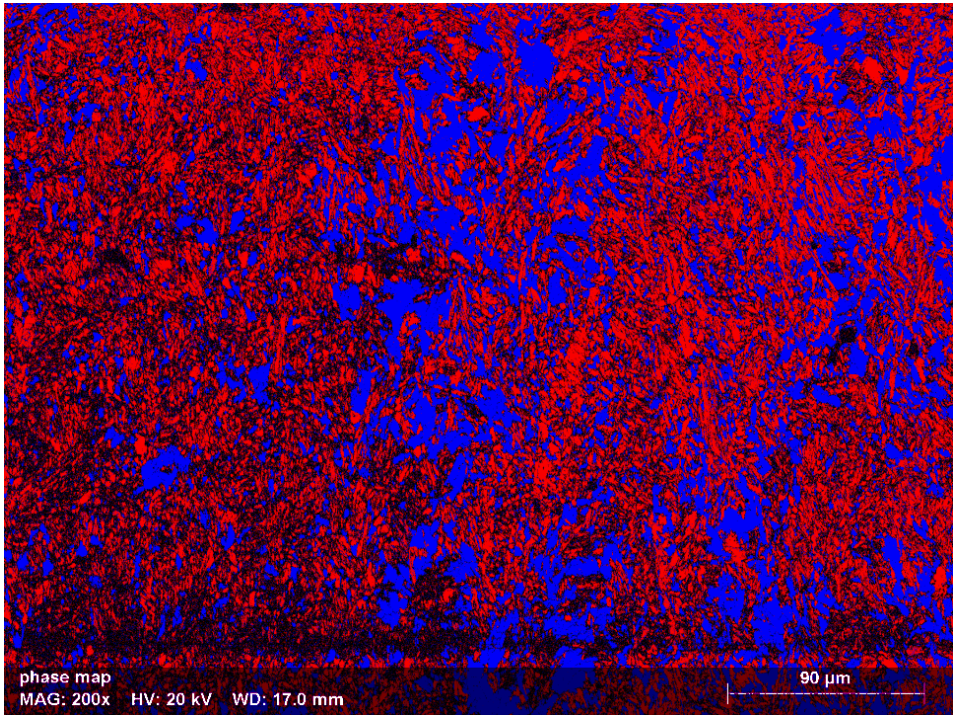


Why Higher Strength for Vendor #2?

- Large fraction of retained austenite exists after solution heat treatment + H900 age
- Conventionally processed 17-4 PH H900 should contain effectively no retained austenite



as-printed



SHT + H900 age

***Blue** = Austenite (FCC), **Red** = Martensite/Ferrite (BCC), **Black** = non-indexed*

Etched Vendor #2 AM 17-4 PH microstructure reveals unexpected solidification features

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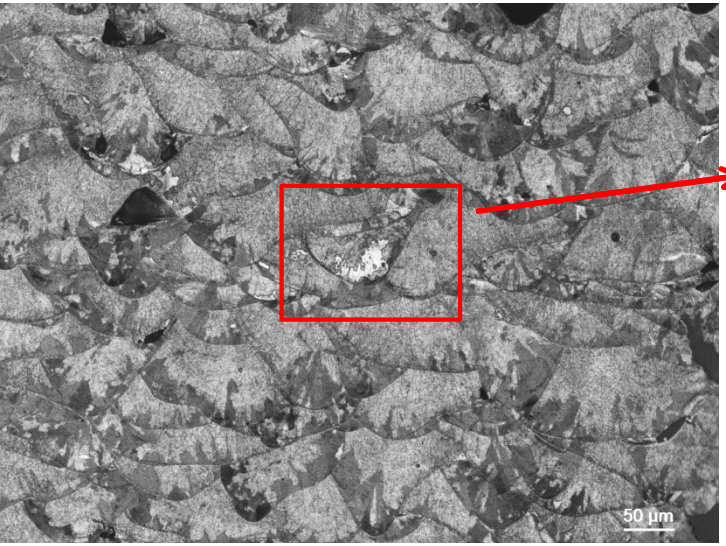
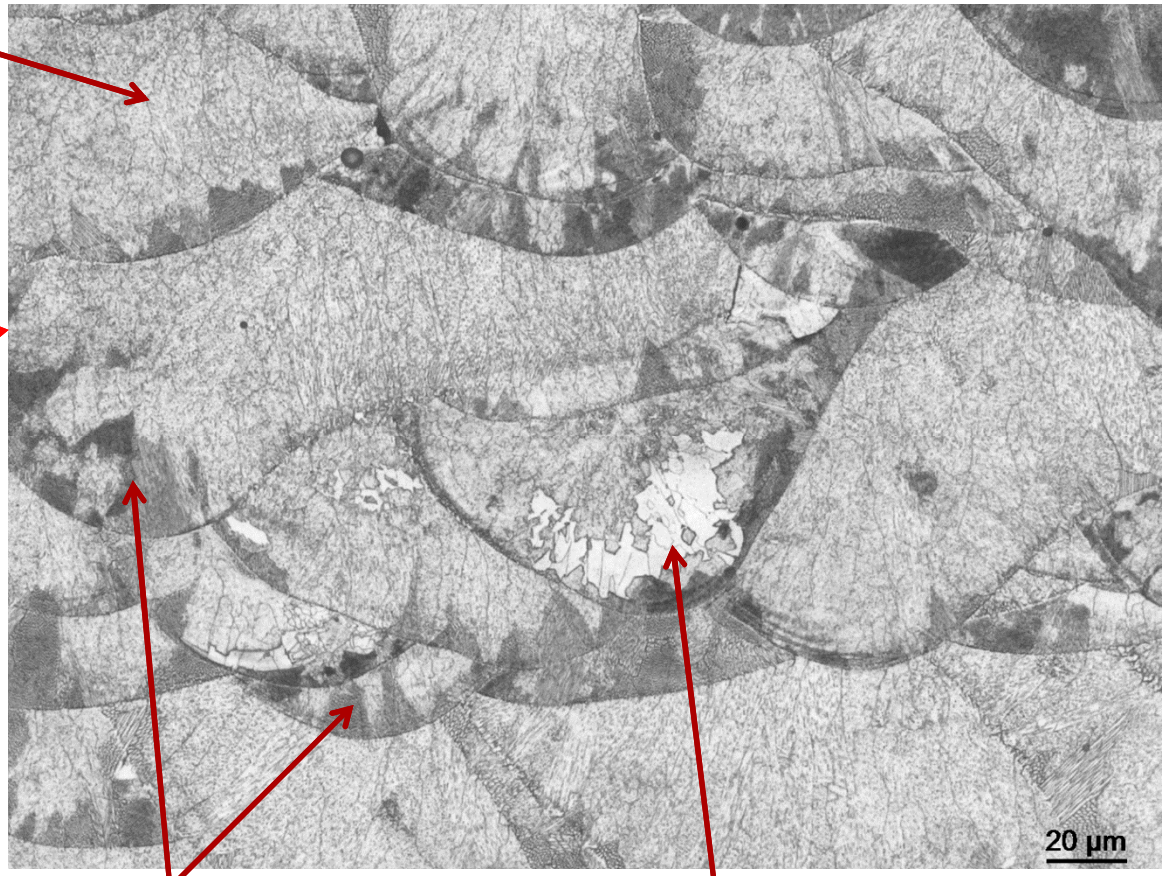
Z

Build Direction

Solidification proceeded as primary ferrite—this is the expected mode for 17-4 PH



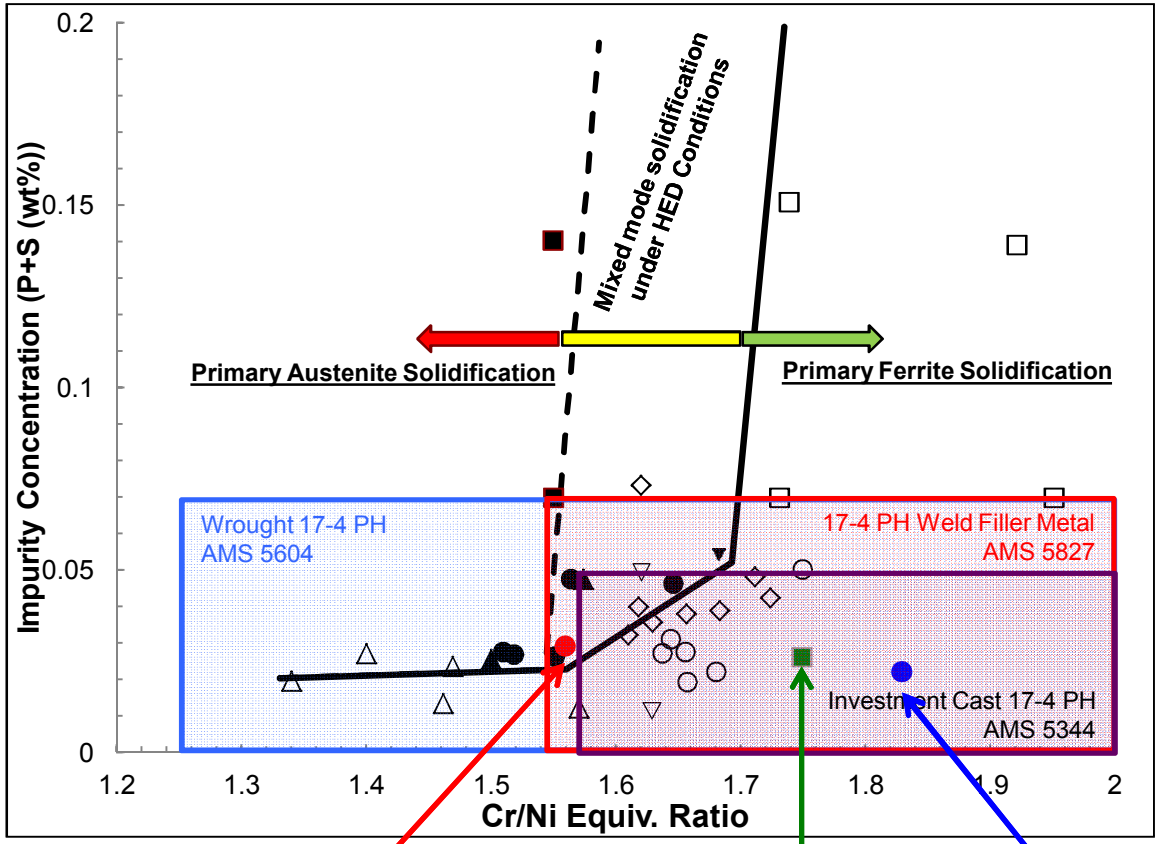


- Unusual mixed-mode solidification observed in Vendor #2 as-printed

Solidification proceeded as primary austenite—**this is NOT the expected mode for 17-4 PH**

Highly Al-rich region; likely contamination

Compositional analysis of AM 17-4 PH shows high austenite stability and propensity for primary austenite solidification for Vendor #2 builds



Vendor #2
M_s: -10°C

17-4 PH sheet
M_s: 109°C

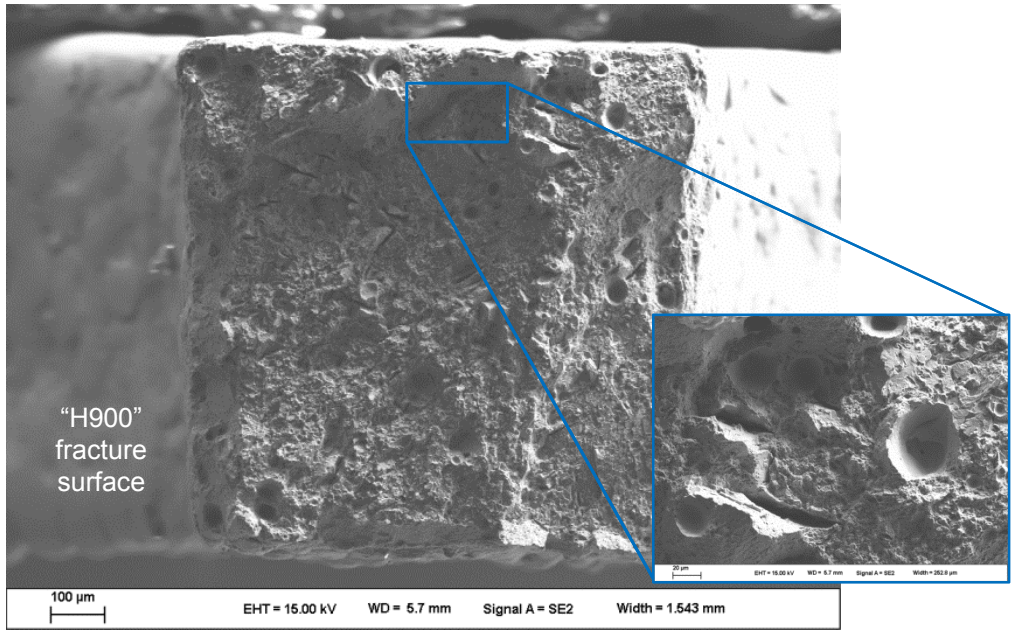
Vendor #1
M_s: 100°C

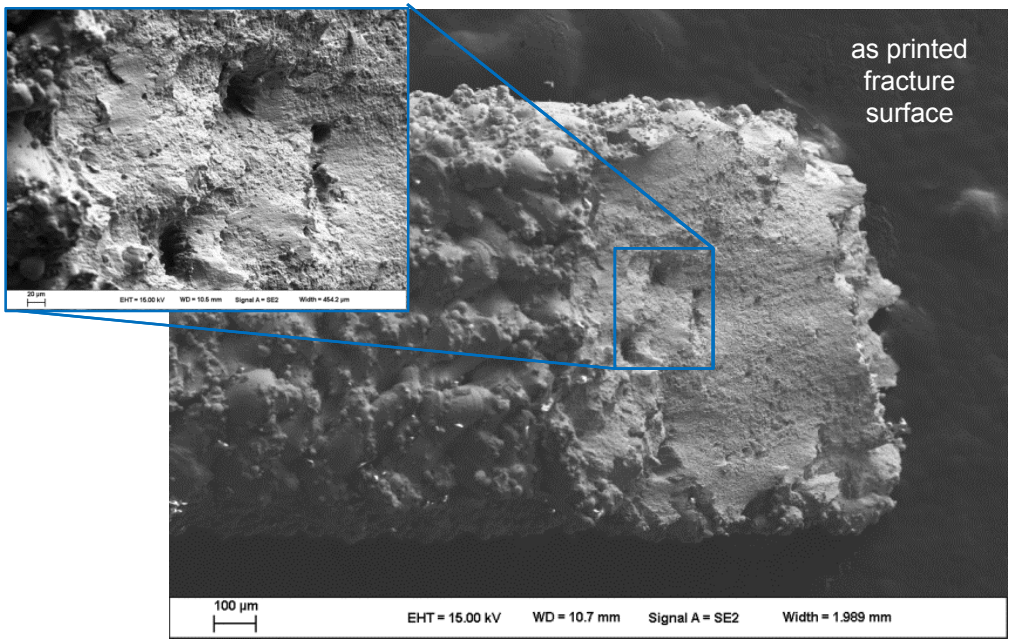
Eichelman & Hull: M_s (°C) = 1302 – 42[Cr] – 61[Ni] – 33[Mn] – 28 [Si] – 1667[C+N]

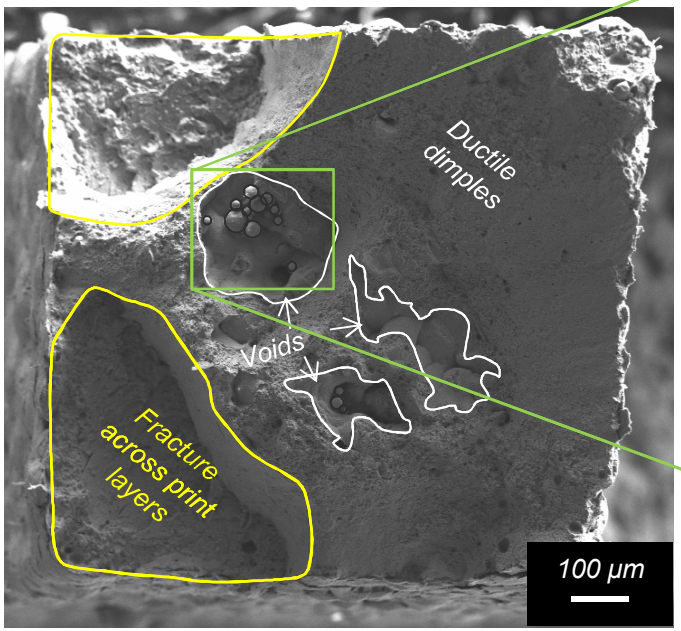
Fractures Suggest Defect Dominated Failure

- "H900"
  - limited area reduction consistent w/"brittle" behavior
  - no clear point of crack nucleation
  - voids at lack-of-fusion boundaries are likely culprits

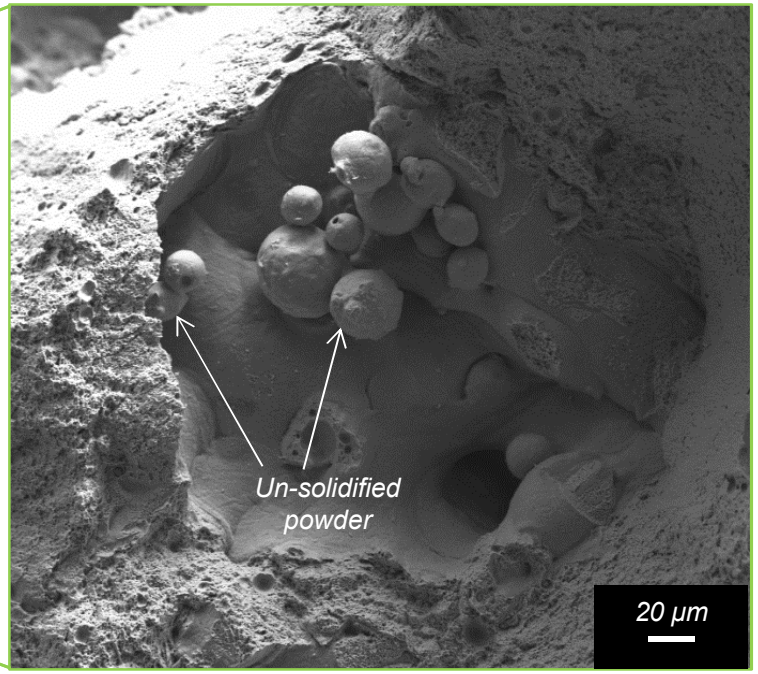
- As printed
  - modest reduction in area
  - surface consistent w/shear-lip tensile failure
    - fine ductile dimples & planes of shear rupture are present
  - spherical particles & voids again suggest lack-of-fusion boundaries as nucleation sites

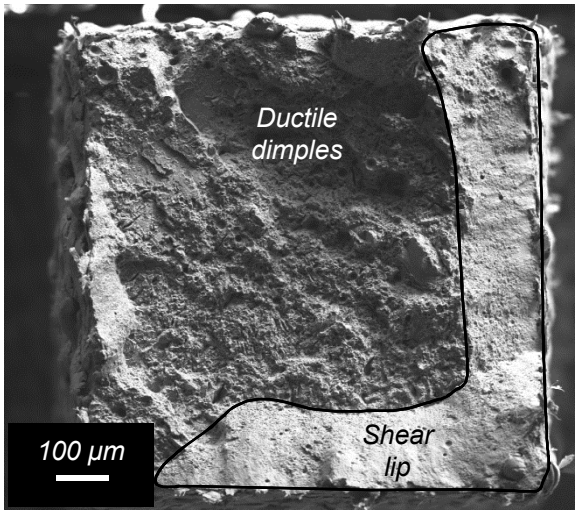






failure at 2% elongation, Vendor 1





failure at 12% elongation, Vendor 1

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QUESTIONS?

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