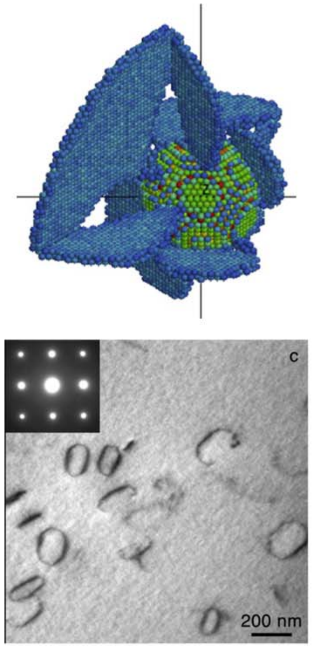
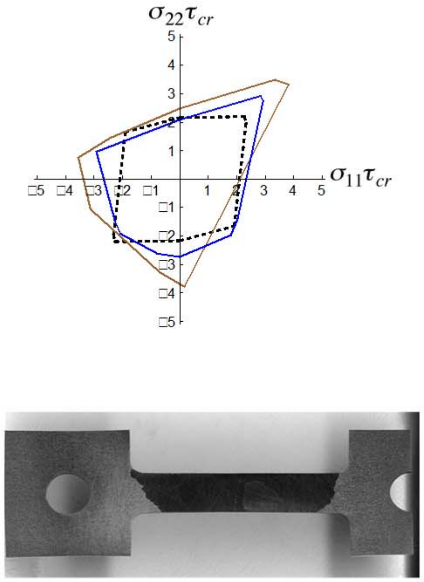
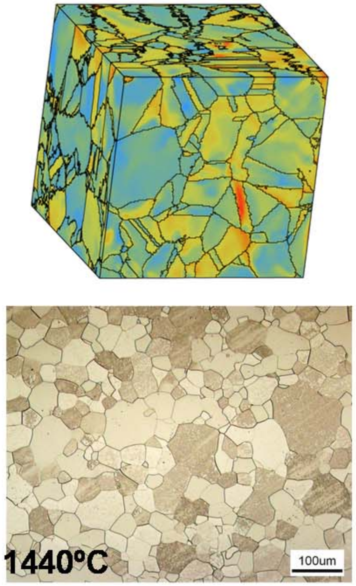
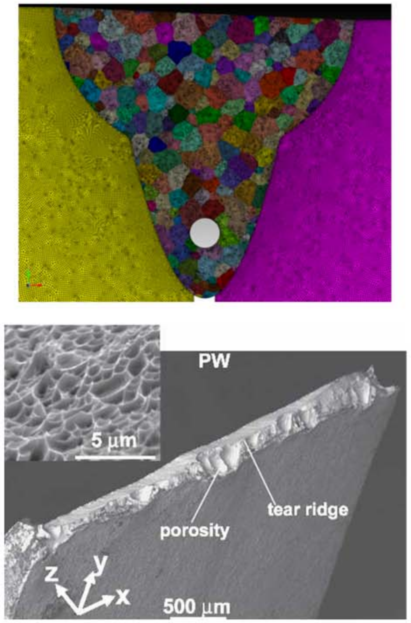
Understand origins of stochastic material response through multiscale materials science







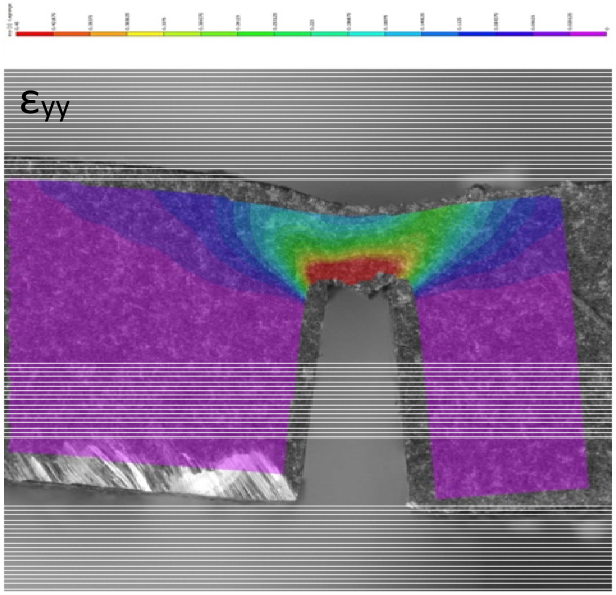


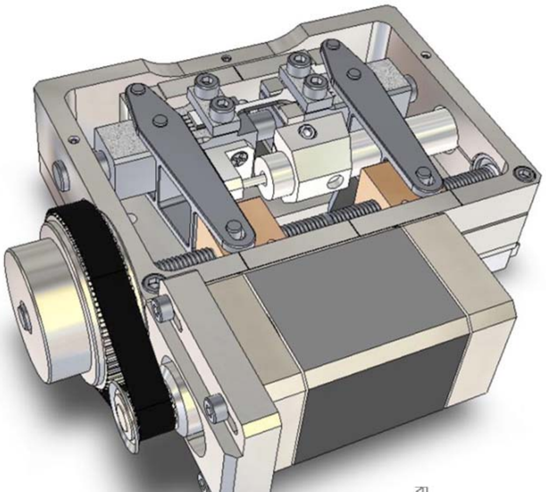
Atomic scale phenomena	**Single crystal behavior**	**Microstructural effects**	**Material performance**
10^{-9} m	10^{-6} m	10^{-3} m	10^{0} m
10^{-9} s	10^{0} s	10^{3} s	10^{6} s

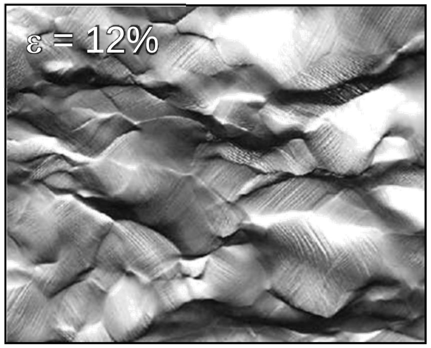
Materials Mechanics Capabilities

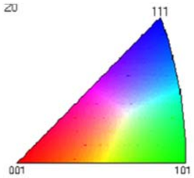
- Roughly $2M in annual programs supported
- 10 MTS Servohydraulic Loadframes
- Extensive traditional extensometry, grips, etc.
- Non-contact laser and LED extensometers
- Digital image correlation strain field mapping, both in optical and electron microscopes.
- Furnaces and thermal cycling chambers capable of -40C to +1400C
- Infrared thermal imaging (up to +1200C)
- Hardness and Charpy testers
- Test timescales from months to milliseconds
- High-speed imaging (up to 250,000 fps)
- Force range of 100 nN to 300 kN
- Specialized, custom capabilities in high-resolution microscale and nanoscale testing:
  - 3 nanoindenters
  - 1 in-situ SEM nanoindenter
  - 1 in-situ SEM tensile stage
  - 2 custom electromechanical probe stations
  - 2 horizontal custom low-force servohydraulic loadframes
  - Extensive optical microscopy facilities, including in-situ optical microscopy

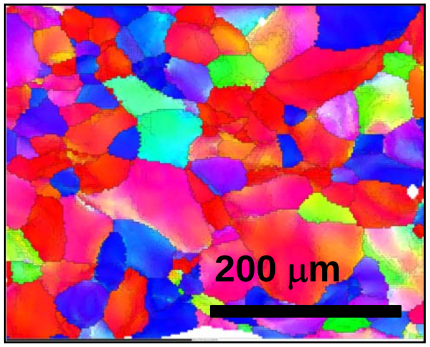
Experimental Materials Mechanics Examples

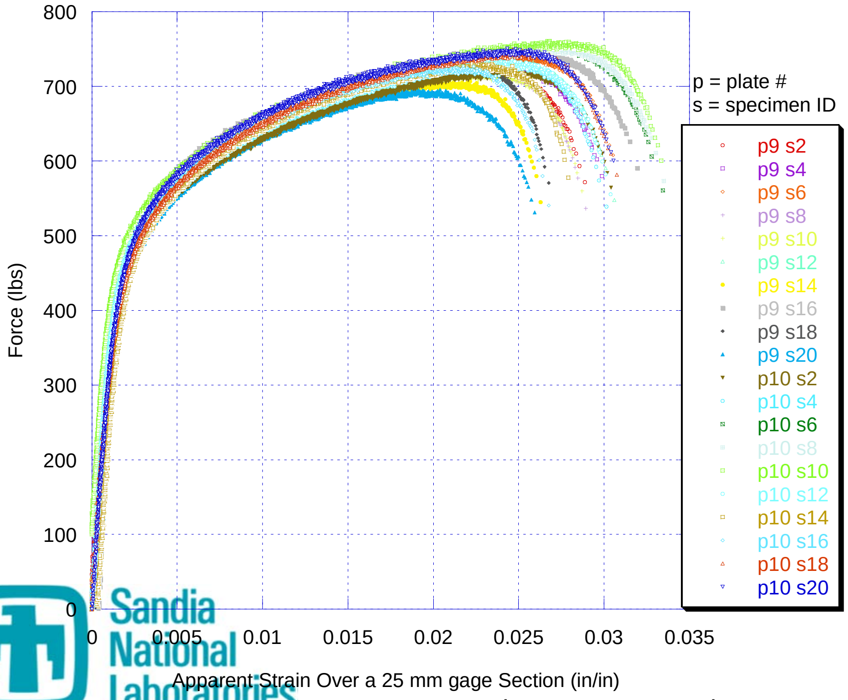


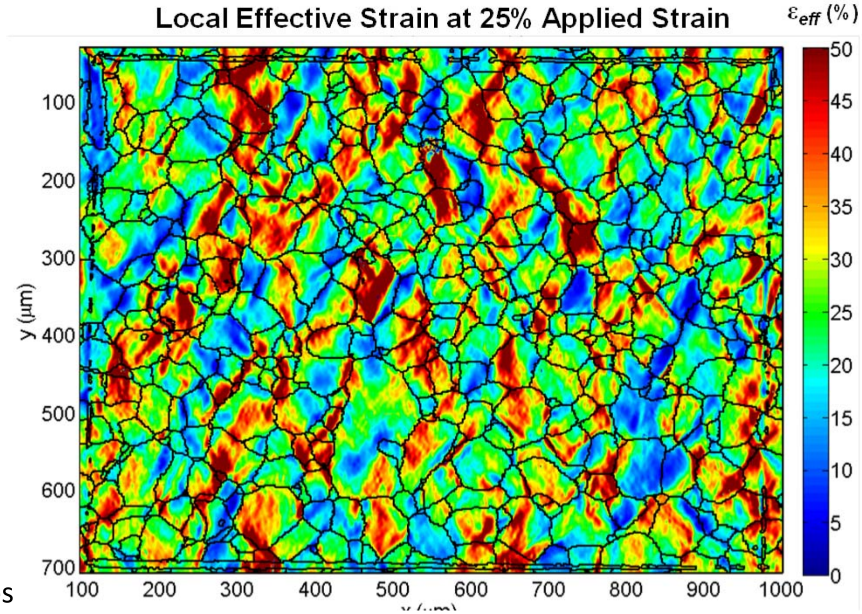








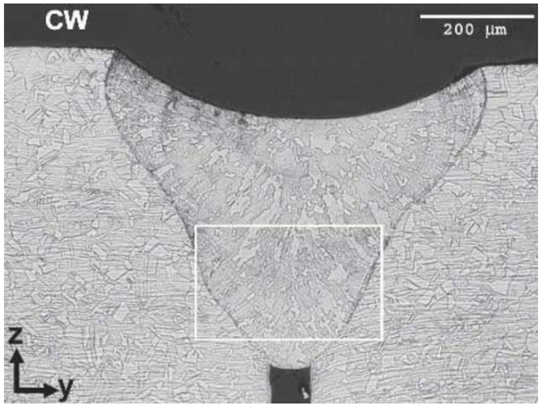


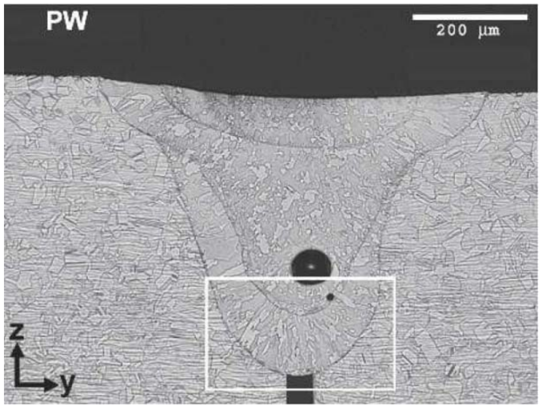


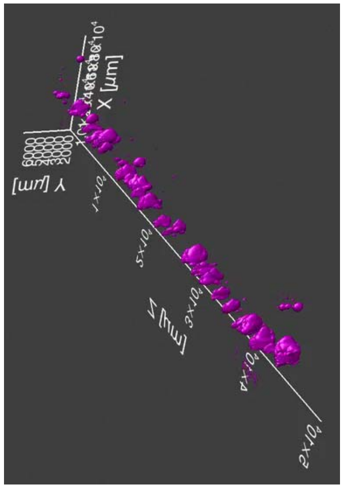
Materials Characterization Capabilities

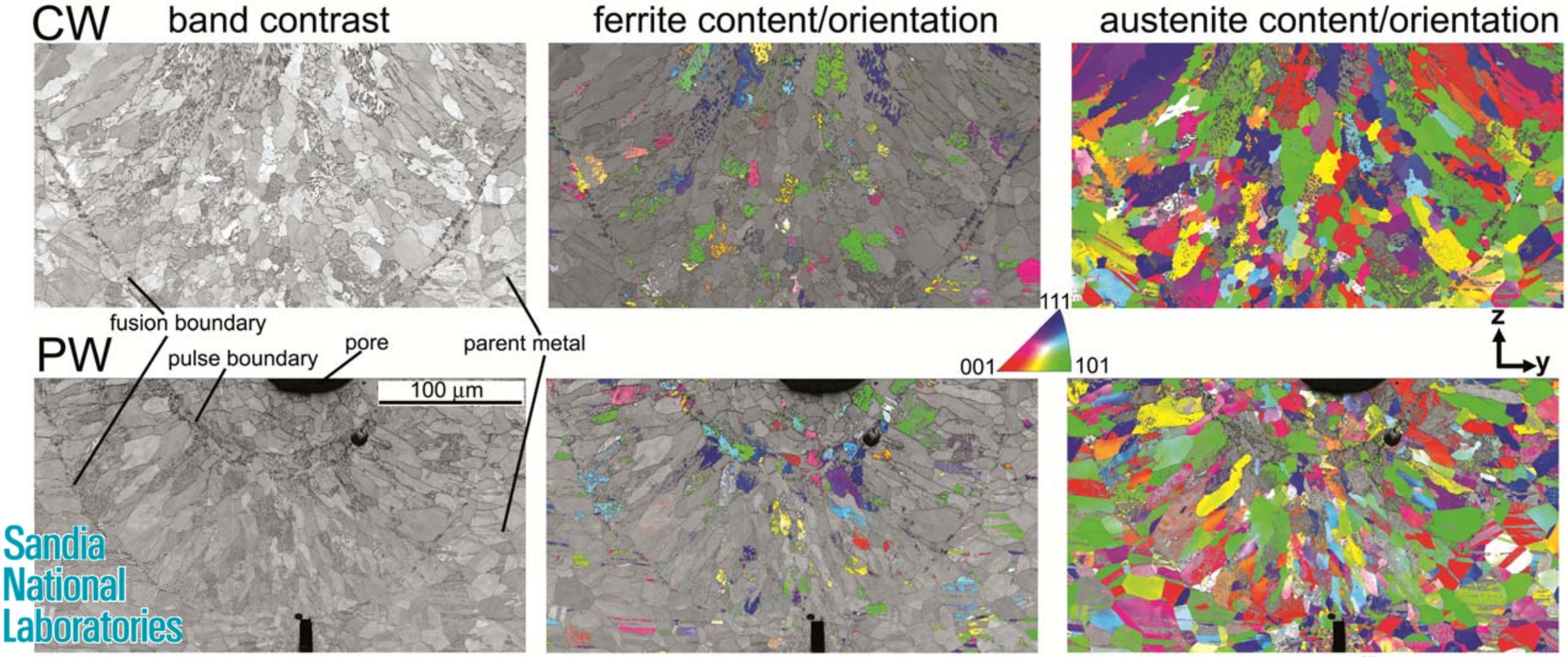
- Extensive metallography suite and highly experienced technicians
- Several field emission scanning electron microscopes with EDS and EBSD capabilities.
- 3 dual-beam focused ion beam electron microscopes with EDS and EBSD capabilities.
- Quantitative microstructural analysis software
- Several transmission electron microscopes with extensive analytic capabilities, EELS, EDS, Spectral Analysis, etc.
- Aberration Corrected scanning transmission electron microscope (probe-corrected)
- X-ray diffraction
- Atomic Force microscope
- Micro x-ray fluorescence capabilities
- Microprobe
- Analytical chemistry lab
- Time-of-flight secondary ion mass spectroscopy
- X-ray/Ultraviolet photoelectron spectroscopy
- Auger electron spectroscopy
- Imaging Near-edge x-ray absorption fine structure
- Nuclear magnetic spectroscopy
- Scanning laser Interferometry
- Failure analysis

Materials Characterization Examples



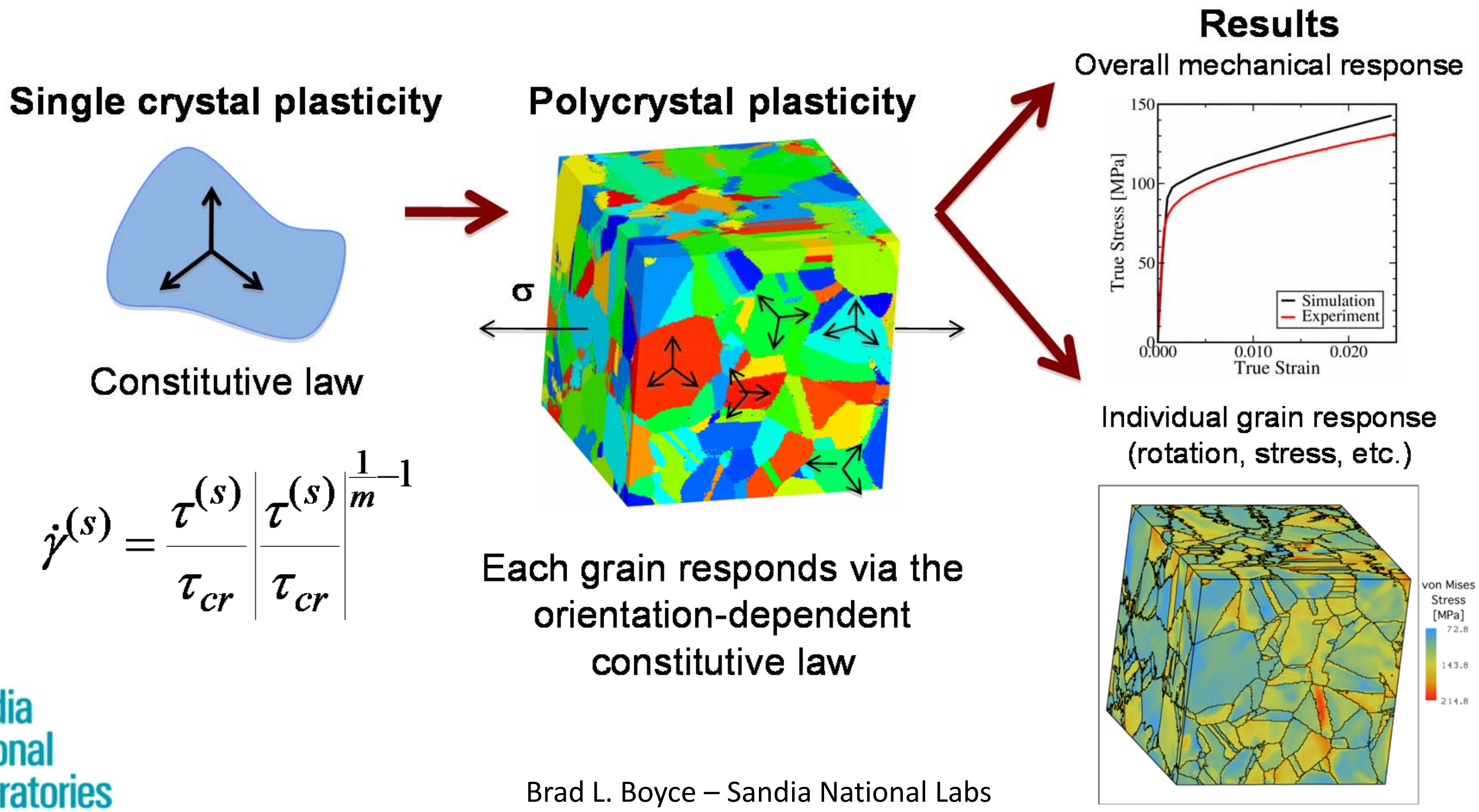






Computational Modeling related to Materials Mechanics

- Ab-initio density functional theory calculations
- Molecular statics and molecular dynamics
- Dislocation dynamics
- Traditional finite element analysis, including coupled thermal-mechanical analysis
- Finite-element representations of material microstructure
  - Polycrystal elasticity
  - Polycrystal plasticity (FCC and BCC metals)
  - Stochastic modeling, including variability in texture, grain morphology, etc.



Single crystal plasticity

Constitutive law

$$\dot{\gamma}^{(s)} = \frac{\tau^{(s)}}{\tau_{cr}} \left| \frac{\tau^{(s)}}{\tau_{cr}} \right|^{\frac{1}{m}-1}$$

Polycrystal plasticity

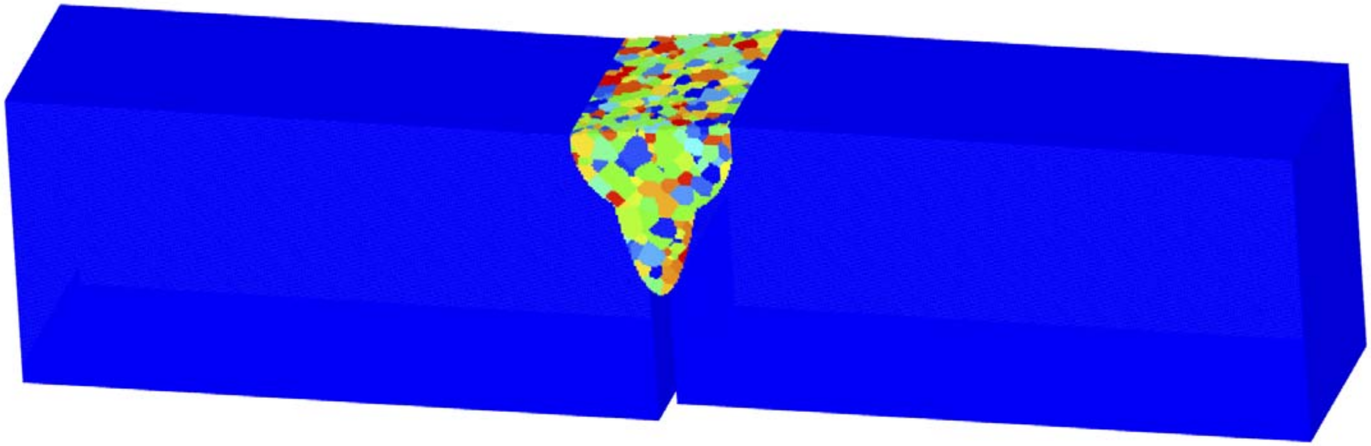
Each grain responds via the orientation-dependent constitutive law

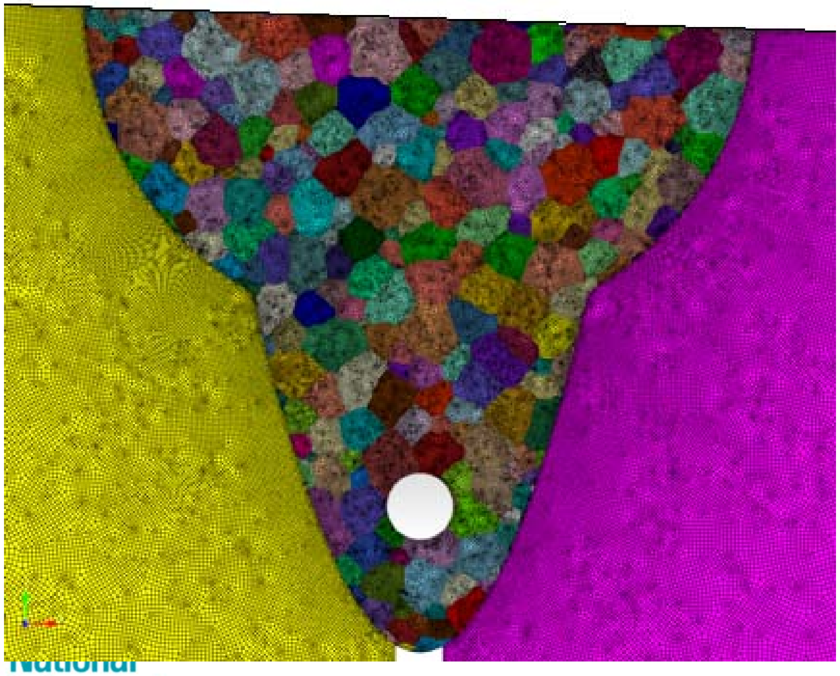
Results

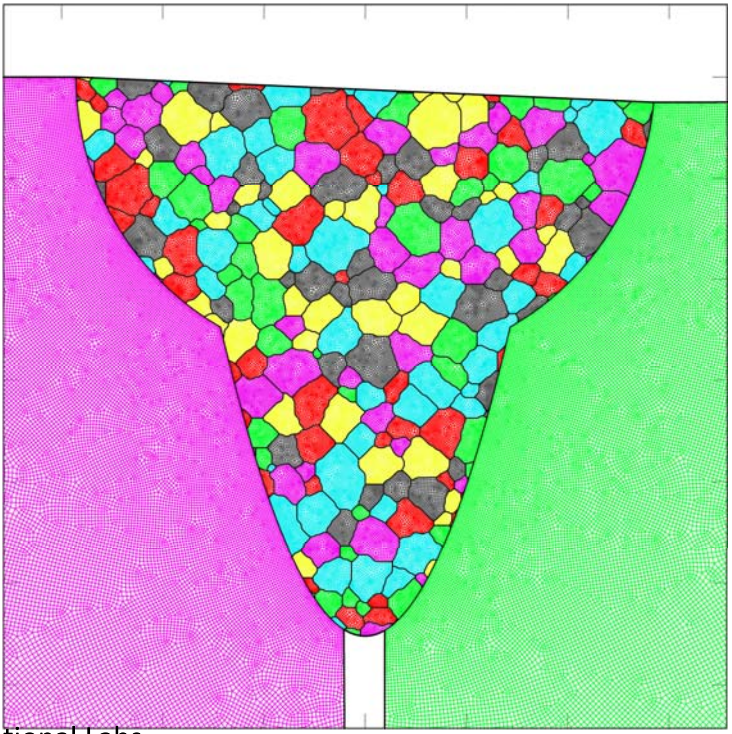
Overall mechanical response

Individual grain response (rotation, stress, etc.)

Computational Materials Mechanics Examples

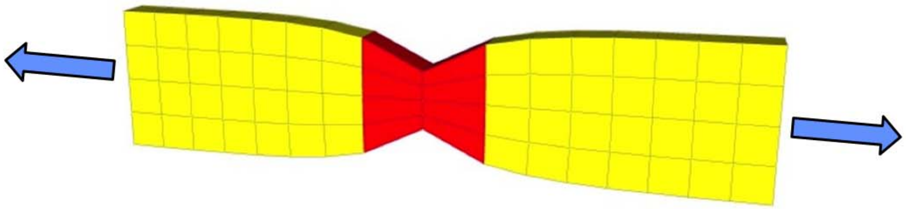


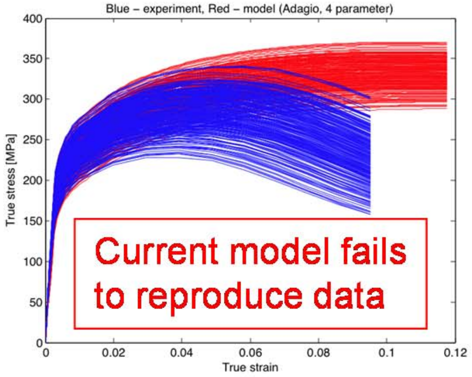




Continuum-down Foundational Problem: Geometric variability in 304L stainless welds

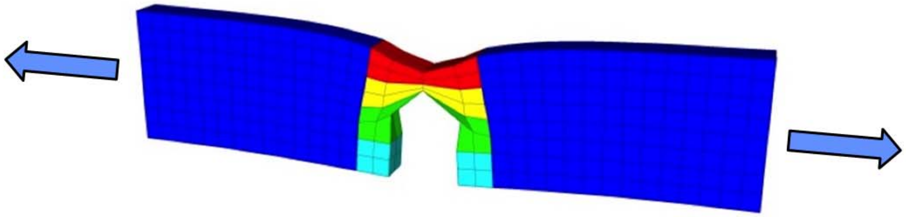
Current design approach: Use a single-material model with 4 parameters; 8 elements per cross-section.

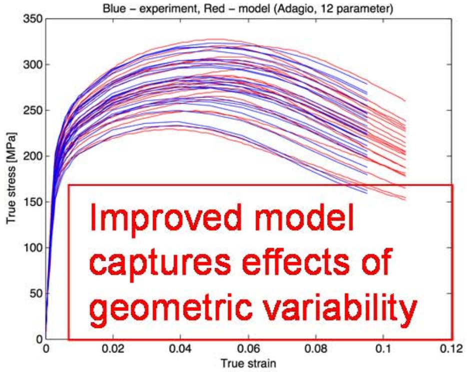




Current model fails to reproduce data

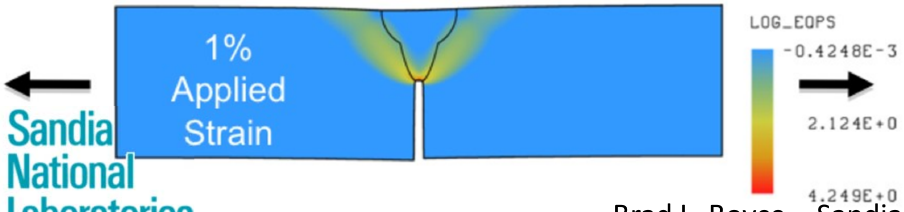
Bridging the gap: Homogenize to 3 material model with 12 parameters; 8 elements with notch per cross-section

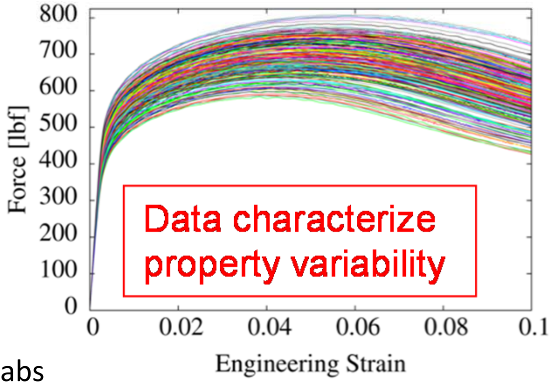




Improved model captures effects of geometric variability

Materials science approach: Computational survey of weld geometries, varying weld depth, plate gap and offset





Data characterize property variability

Some representative publications related to stochastic/microstructural mechanics
(see pdf's sent previously)

Buchheit2005: A paper detailing the formulation for polycrystal plasticity for FCC metals. This framework has also been used for problems of elasticity. It includes a complete anisotropic representation of the elastic constants for each grain in a polycrystal.

Counts2008: Elastic properties homogenized from atomic scale to FEM scale (work largely done in Germany, with collaboration with Sandia)

Counts2008b: Modeling grain boundary hardening in a polycrystal plasticity framework.

Brewer2009: An example of the integration of experimental materials characterization such as EBSD with computational modeling such as polycrystal plasticity to understand mechanical behavior.

Battaile2009: Using brass as a simple material system, we use electron backscatter diffraction, digital image correlation, and polycrystal plasticity modeling to understand the role of microstructure on the mechanics of a deforming hole in a tensile bar.

Boyce2009: An example of some of my past work on understanding the strain-rate sensitivity of tensile behavior in several steel alloys. Modulus was not a concern in that previous study.

Boyce2010: An example in silicon microsystems of very small tensile bars used to generate large statistical datasets, in this case of fracture strength.

Dingreville2010: Ways to represent real microstructure into a polycrystal FEM framework.

Buchheit2011: Extending our existing FCC polycrystal plasticity model to represent BCC metals; there is a full paper in preparation.