SAND2013-1814P

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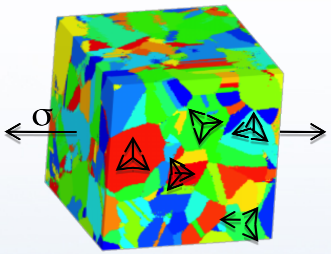

Predicting Performance Margins

Uniting experimental and computational materials science tools to improve statistically-informed engineering design

Status Update --January 2013

Brad L. Boyce (1831)

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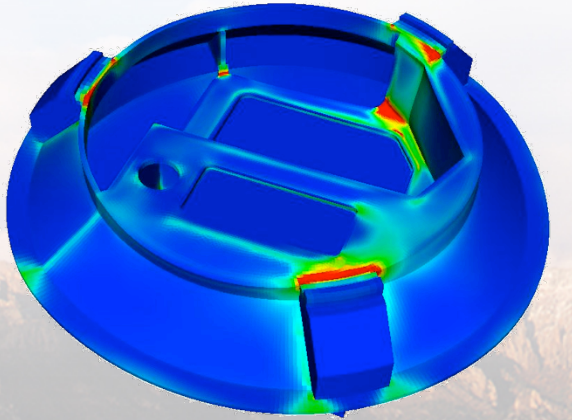
Mechanical Nuclear Safety Performance is a PPM Driver

Loading accidents

Predictive capabilities are needed during design and qualification to ensure failure does not occur under normal or abnormal environments.

SGT crash

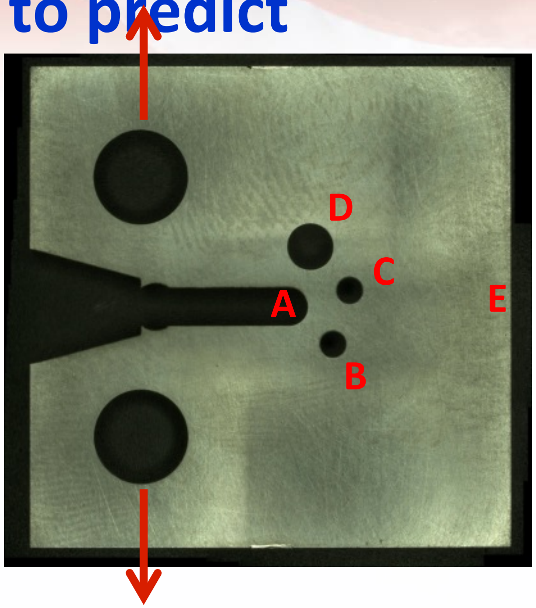
Predicting Weld Failure



Failure of metals is difficult to predict

The 2012 Sandia Fracture Challenge: In the notched C(T) geometry shown, predict the force-displacement curve associated with crack initiation and crack propagation.

(Details on geometry and alloy (15-5 PH) provided including tensile and fracture toughness tests)



- Liang Xue / **Schlumberger**
- Andrew Gross, Ali Ghahremaninezhad*, K. Ravi-Chandar **/ University of Texas at Austin**, University of Miami
- Tomasz Wierzbicki, Meng Luo, and Keunhwan Pack / **Massachusetts Institute of Technology**
- Mike Neilsen, Kristin Dion, Amy Kaczmarowski, Erin Karasz / **Sandia** computational solid mechanics
- J. S. Chen, Shih-Po Lin, Edouard Yreux, Marcus Rüter, Sheng-Wei Chi / **University of California, Los Angeles**
- Dong Qian[1], Zhong Zhou, Sagar Bhamare / University of Cincinnati [1] Currently at the University of Texas at Dallas
- Steffen Brinckmann, Lukas Quinkert / ICAMS, **Ruhr-University Bochum**
- Shan Tang, Khalil Elkhodary, Jifeng Zhao, Devin O'Connor and Wing Kam Liu / **Northwestern University**
- Anthony Ingraffea, Bruce Carter, Paul Wawrzynek, Albert Cerrone, John Emery, Michael Veilleux, Jacob Hochhalter / **Cornell**-led team (with Sandia, NASA)
- Pengfei Yang[1] , Yong Gan[2], Xiong Zhang[1], Zhen Chen[3] / [1]Tsinghua University, [2]Zhejiang University, **[3]University of Missouri** and Dalian University of Technology
- Erdogan Madenci and Bahattin Kilic, **University of Arizona**
- Jim Lua / **Global Engineering and Materials**
- Tom Moyer, Ken Nahshon, Ray Defrese, Michael Miraglia, Jamie Rankin / **Naval Surface Warfare Center** Carderock Division (NSWCCD)
- Junhang Guo, **Xi'an Jiaotong University**

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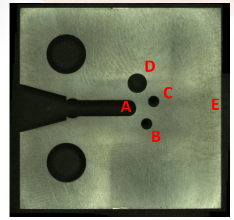
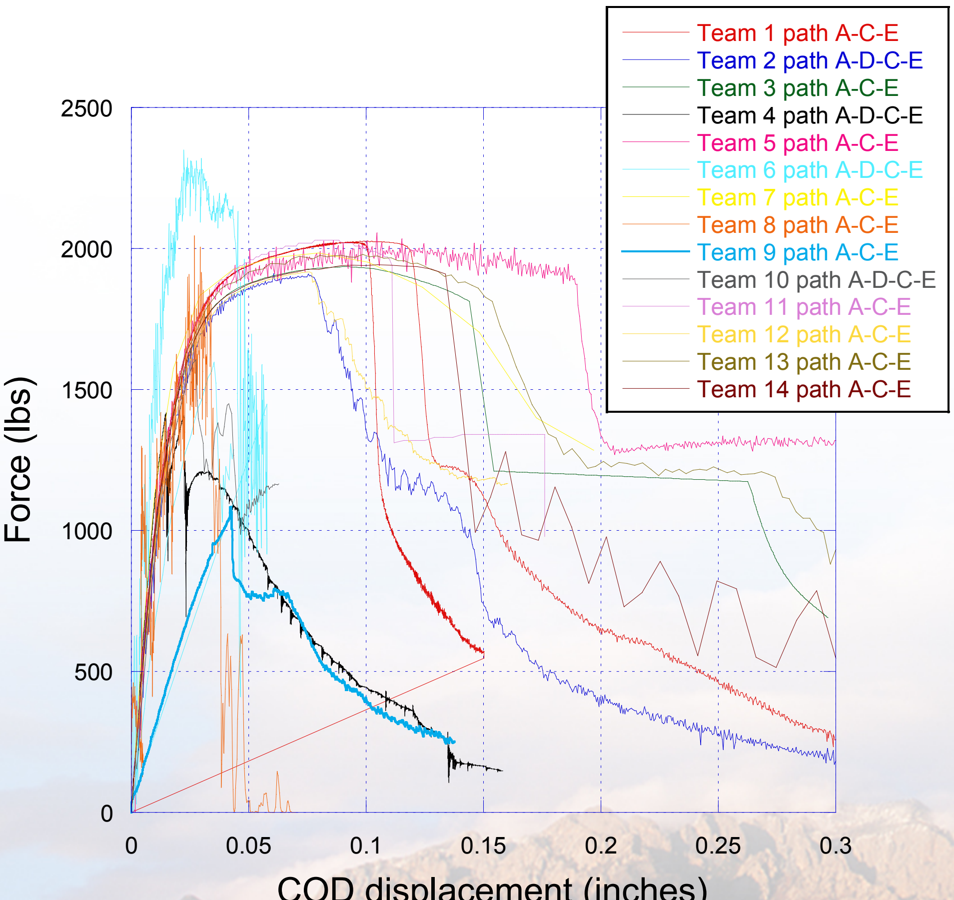
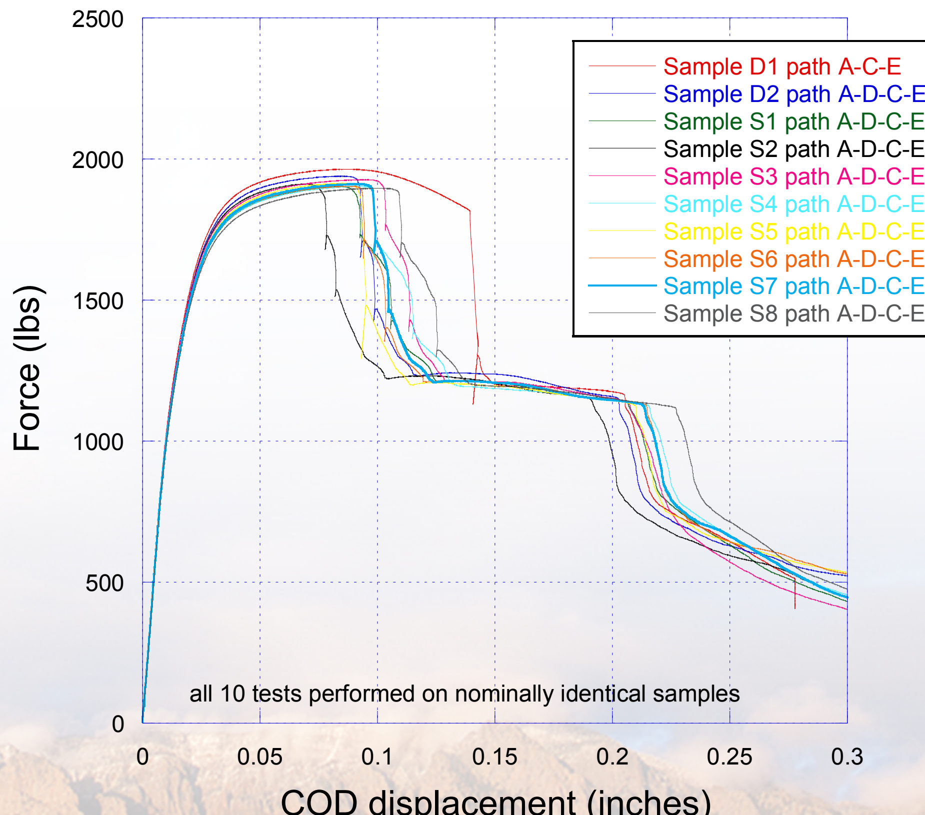
Failure of metals is difficult to predict



predictions - 14 institutions



experiments - Sandia solid mechanics
Sharlotte Kramer and Theresa Cordova



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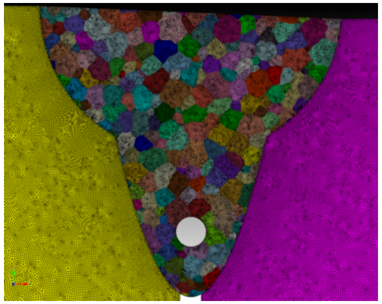
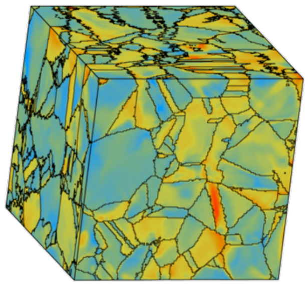
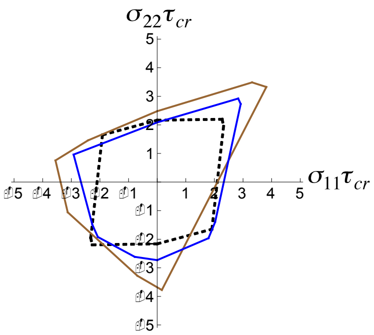
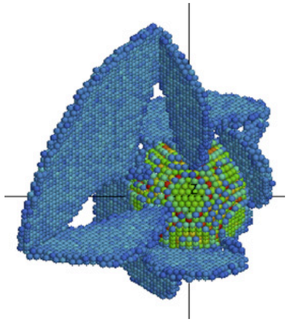
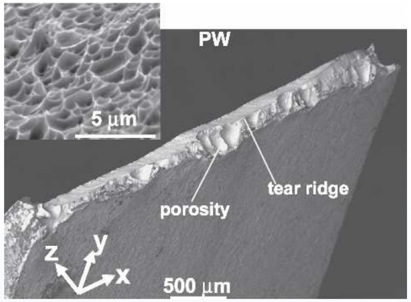
PPM integrates models and tools using continuum-down and atoms-up approaches

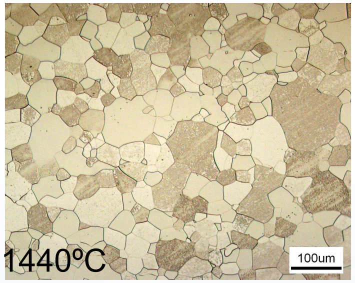


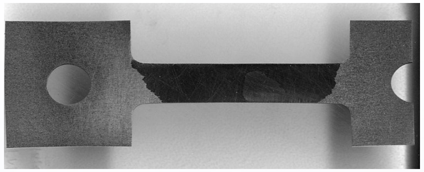


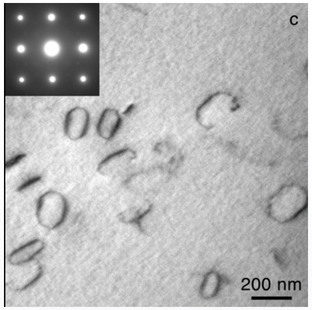












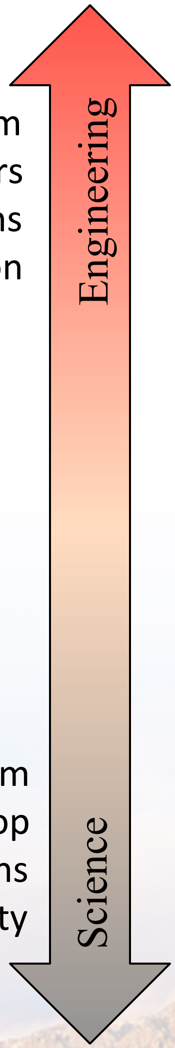
Material performance	Microstructural effects	Single crystal behavior	Atomic scale phenomena
10^{0} m 10^{6} s	10^{-3} m 10^{3} s	10^{-6} m 10^{0} s	10^{-9} m 10^{-9} s

Atoms-up: Develop physics-based models to provide scientific insight

Continuum-down: Augment engineering-scale models to provide customer value

There is a spectrum of interrelated questions spanning from engineering application to basic science

Short-Term
Need fast answers
Use existing equations
Specific to Application

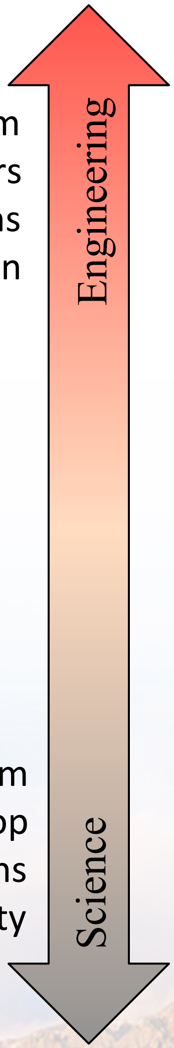


Long-term
Slow to develop
Derive new equations
Broad Applicability

- Will component X fail under a certain environment?
- How much margin exists between operation and failure?
- What is the probability that component X will fail in a certain environment?
- How consistent & homogeneous is the material and manufacturing processes?
- What is the mechanism by which failure occurs?
- What is the governing equation that dictates failure? Can the failure process be modeled, simulated, and predicted based on knowledge of the material & manufacturing processes?

There is a spectrum of interrelated questions spanning from engineering application to basic science

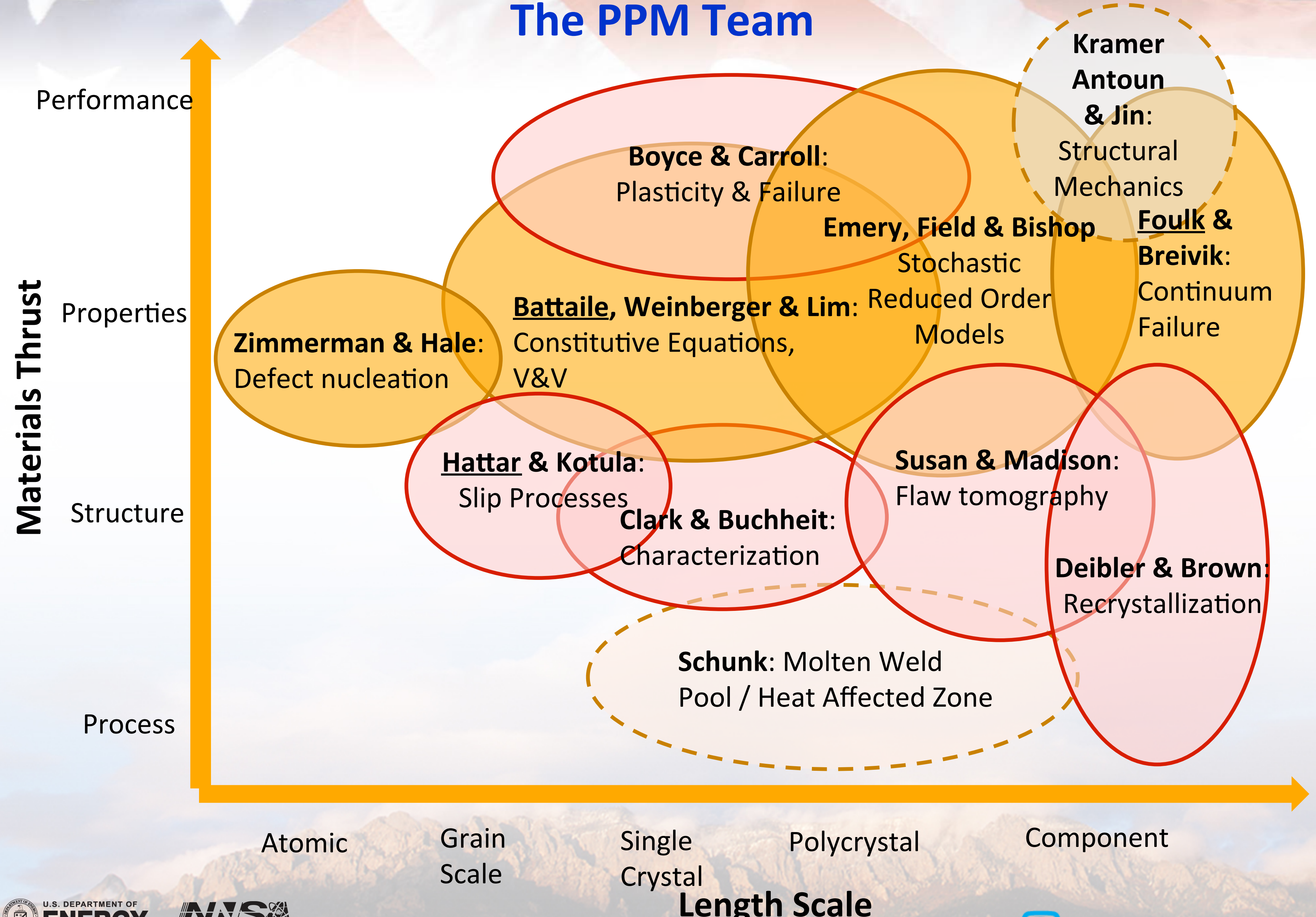
Short-Term
Need fast answers
Use existing equations
Specific to Application



Long-term
Slow to develop
Derive new equations
Broad Applicability

- How do we specify the allowable degree of porosity in laser welds for a fireset housing?
- How do we represent micro-scale porosity in a finite element model to predict real component failure?
- How do pores affect the strength and ductility of metals?
- How do pores interact with microstructure: grain boundaries, precipitates, second phases, prior cold work, chemical segregation, etc.
- What is the mechanism and constitutive equation governing crack nucleation in ductile metals?
- How does atomic-scale dislocation slip progress in BCC metals, and how does this vary as a function of temperature and strain-rate?

The PPM Team



Materials Thrust
Performance
Properties
Structure
Process
Kramer Antoun & Jin: Structural Mechanics
Boyce & Carroll: Plasticity & Failure
Emery, Field & Bishop Stochastic Reduced Order Models
Foulk & Breivik: Continuum Failure
Zimmerman & Hale: Defect nucleation
Battaile, Weinberger & Lim: Constitutive Equations, V&V
Hattar & Kotula: Slip Processes
Clark & Buchheit: Characterization
Susan & Madison: Flaw tomography
Deibler & Brown: Recrystallization
Schunk: Molten Weld Pool / Heat Affected Zone
Atomic
Grain Scale
Single Crystal
Polycrystal
Component
Length Scale

PPM connects young staff with seasoned veterans and NW customers

Task 1: Nanoscale framework for crack initiation and growth

J Zimmerman (8246), C Weinberger (1814), P Kotula (1822), K Hattar (1111), L Hale (8246)

Task 2: Microscale effects of defect fields

B Boyce (1831), C Battaile (1814), B Clark (1111), T Buchheit (1814), J Puskar (1822), J Carroll (1831), H Lim (1814), L Deibler (1822)

Task 3: Connecting microstructural variability to performance margins in structural metals

J Emery (1524), A Brown (8259), J Foulk (8256), R Field (1526), D Susan (1822), J Madison (1814)

Technical Advisory Council

S Foiles (1814), N Breivik (1524), R Hogan (1514), D Medlin (8656), J Michael (1822), N Moody (8222), M Nielsen (1526), D Reedy(1526), C Robino (1831)

Customer Advisory Council

R Paulsen (2211) (chair), D Balch (8224), E Fang (1524), R Oetken (8244), T Mattsson (1641), J McLaughlin (0425), A Roach (2735), R McCormick (1110), T Trinh (2547), S Kempka (1510), J Johannes (1520)

External Collaborators

LLNL, LANL, UT Austin, Michigan State University, Georgia Tech, General Motors, Caltech, Cornell, Carnegie Mellon, etc.

Metrics for Success

6 Sandia design & production efforts that are utilizing PPM expertise

6 international symposia organized on PPM-related topics

>15 invited/keynote presentations given at major conferences

9 journal articles published including an invited review article

1. T.E. Buchheit, C.C. Battaile, C.R. Weinberger, and E.A. Holm, "Multi-scale modeling of low-temperature deformation in B.C.C. metals", *JOM*, 63(11), p. 33-36, 2011.
2. C.R. Weinberger, C.C. Battaile, T.E. Buchheit, and E.A. Holm, "Incorporating atomistic data of lattice friction into BCC crystal plasticity models", *International Journal of Plasticity*, 37, p. 16-30, 2012.
3. J.D. Carroll, L.N. Brewer, C.C. Battaile, B.L. Boyce, J.M. Emery, "The effect of grain size on local deformation near a void-like stress concentration", *International Journal of Plasticity*, 39, p. 46-60, 2012.
4. J. Madison, L. K. Aagesen, "Quantitative Characterization of Porosity in Laser Welds of Stainless Steel," *Scripta Materialia*, 67(9), p. 783-786, 2012.
5. **[invited]** C.R. Weinberger, B.L. Boyce, and C.C. Battaile, "Slip planes in BCC transition metals", accepted for publication in *International Materials Reviews*, November 2012.
6. B.L. Boyce, B.G. Clark, P. Lu, J.D. Carroll, and C.R. Weinberger, "The morphology of tensile failure in tantalum", submitted to *Metallurgical and Materials Transactions A*, June 2012.
7. C.R. Weinberger, G.J. Tucker, and S.M. Foiles, "The Peierls potential of screw dislocations in BCC transition metals: predictions form density functional theory", submitted to *Physical Review B*, December 2012.
8. H. Lim, C. R. Weinberger, C .C. Battaile, T. E. Buchheit, "Application of generalized non-Schmid yield law to low temperature plasticity in BCC transition metals", submitted to *Modeling and Simulation in Materials Science and Engineering*, November 2012.
9. J.D. Carroll, B.G. Clark, T.E. Buchheit, B.L. Boyce, and C.R. Weinberger, "An experimental statistical analysis of stress projection factors in BCC tantalum", submitted to *Materials Science and Engineering A*, February 2013.

Communication is the backbone for PPM

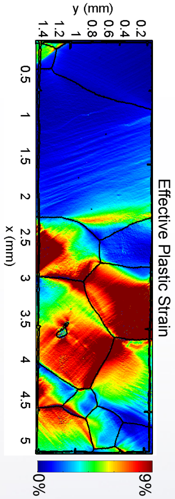
- Chris Deeney briefing at Sandia in October, 2011.
- NA-11 seminar in January 2012 (Chris Deeney and Robert Hanrahan).
- Annual update to CTO in 2011, 2012, and 2013.
- Technical advisory board briefing and customer advisory board briefing held in 2011 and 2012.
- Center 2100/8200 Weapons S&T Seminar Series showcased PPM in August and September 2012.
- Paul Hommert, Don Cook, and Gary Sanders have all been briefed on PPM during 2012.
- In October 2012, a full-day on-site Summit was held to foster communication among team members and university collaborators.

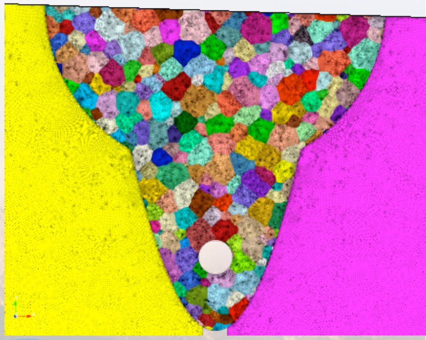
PPM Impact to NW Programs

- **Inform material-science & engineering decisions**
  - Systems designs: W88-ALT and B61-12 LEP
  - Troubleshooting:
    - 304L non conforming tubing: B83-ALT 353
    - Power source rupture
    - Weld failure: W88-ALT drop tests
  - Manufacturing support
  - Surveillance support
- **Prototype for other NW needs**
  - Glass-to-metal seals
  - Active brazing

PPM Impact to NW Programs

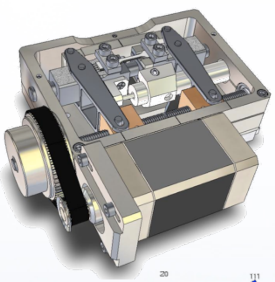
- **Foundational capability enhancement**
  - **Research**
    - Staff development
      - **Sustained, focused research opportunity, support individual initiative, expand NW contacts, provide project leadership opportunities**
    - Knowledge base
      - **Foster new capabilities, propagate corporate knowledge, provide foundation for science-based requirements and future NW customer support**
  - **Develop Experimental Capabilities**
    - 3D material characterization
      - **Microscopy, FIB, RoboMET, tomography, digital image correlation**
    - Advanced testing capabilities
      - **in-situ quantitative nano/microstructural scale deformation, multi-axial weld test capabilities**
  - **Develop Modeling and Simulation Capabilities**
    - Codes
      - **SM/SD, MD, SIERRA framework**
    - Models
      - **Physical models, constitutive relations, reduced-order modeling, microstructure-informed predictions**

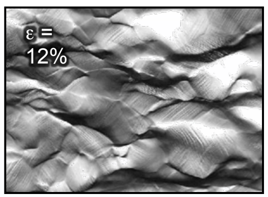


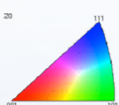


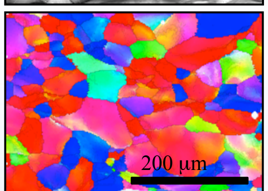
Advanced Capabilities for All NW Needs

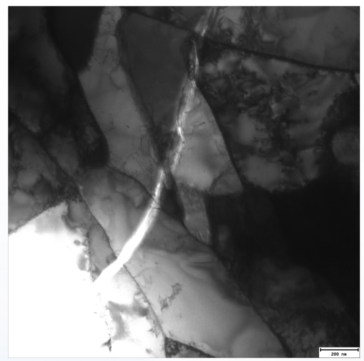
- **Modeling**: atomistic, single crystal, polycrystal, weld variablity, porosity, weld performance…
- **Experimental**: microscopy (TEM, SEM, EBSD, RoboMet™), microtomography, single- and oligocrystal growth, digital image correlation, *in situ* testing, advanced mechanical testing, …

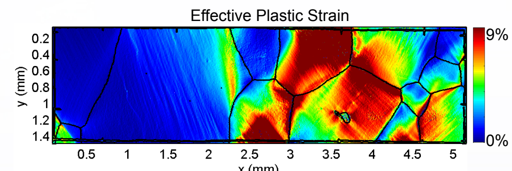


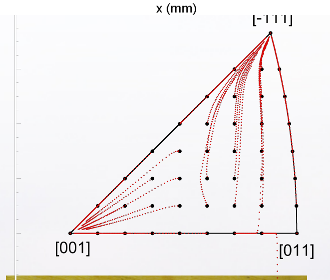


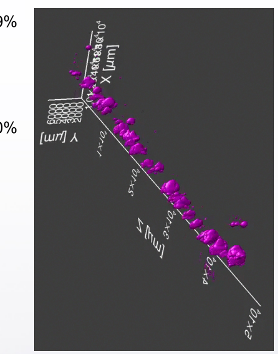


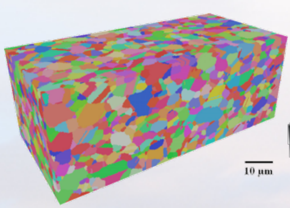


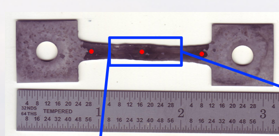


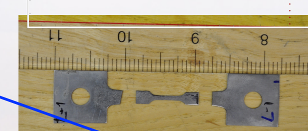


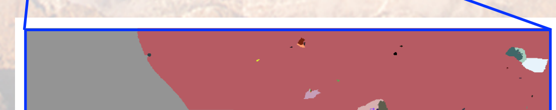












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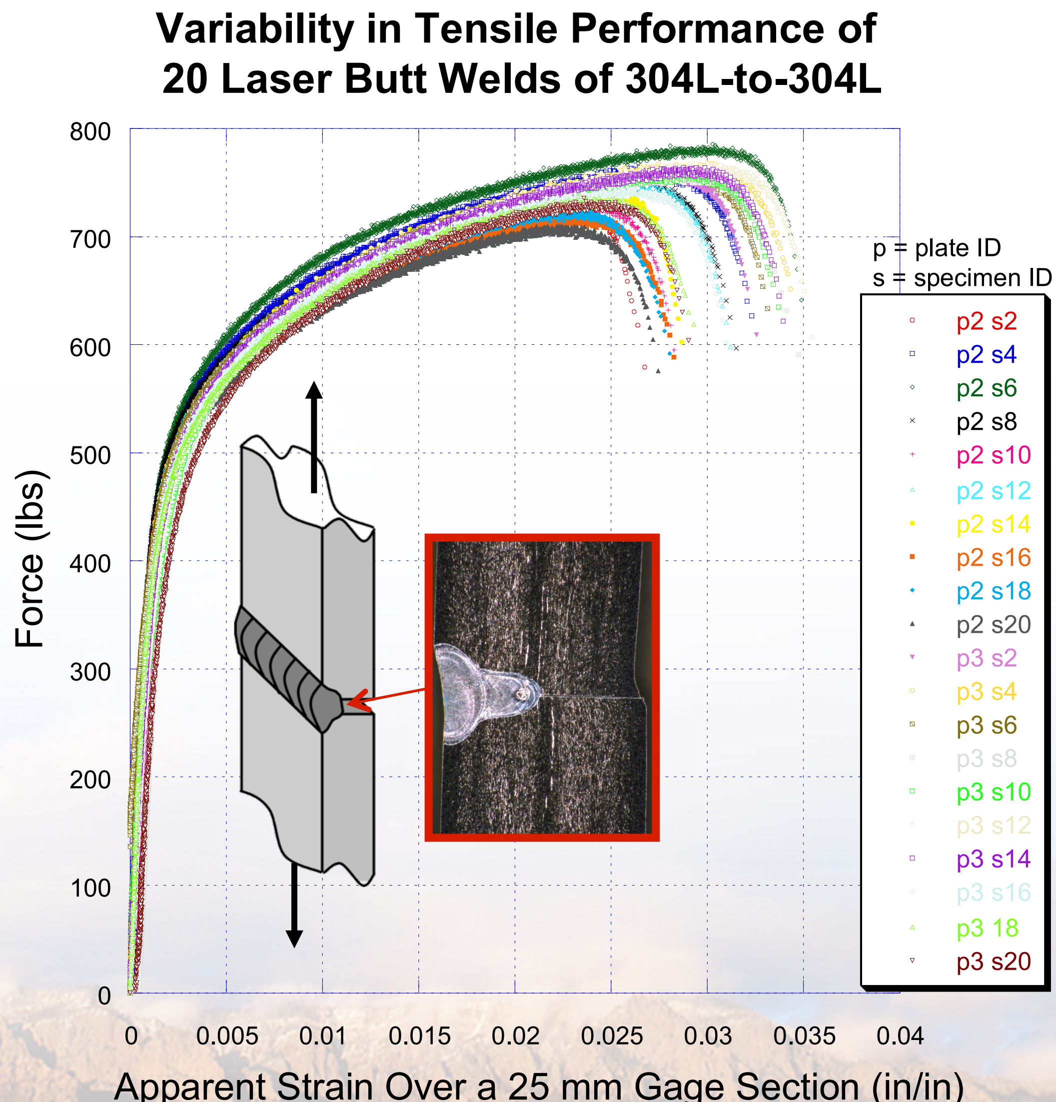
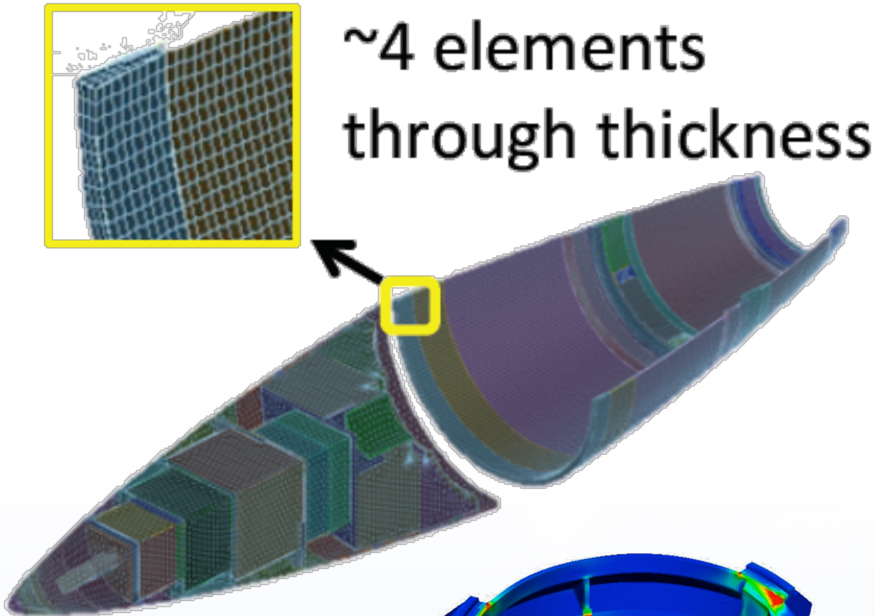
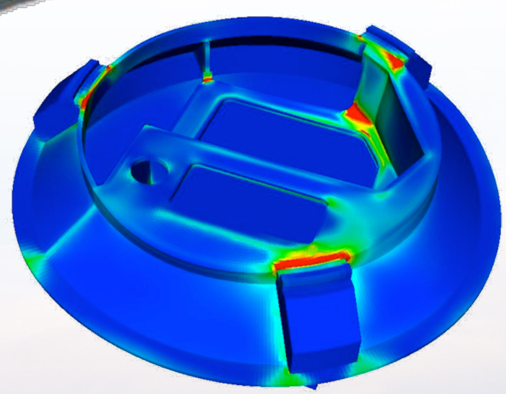
Weld performance is highly stochastic

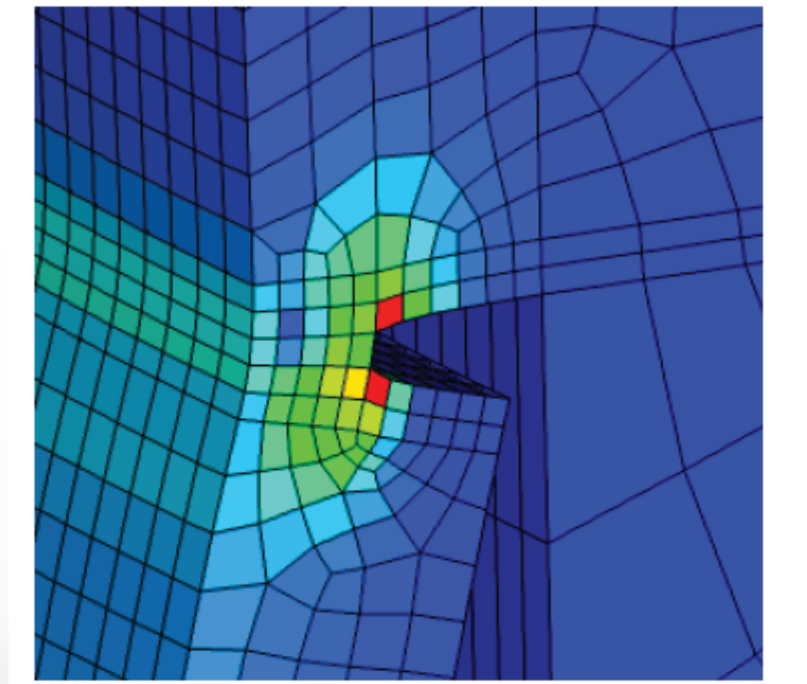
- Previous experience had shown that the porosity content was strongly affected by the choice of laser welding process: pulsed-wave (PW) welding produced significant porosity whereas continuous-wave (CW) produced very litte porosity.
- 20 tensile bars containing laser welds were tested: 10 with the CW process (low porosity) and 10 with the PW process (high porosity).
- A wide degree of variability was observed in the force-displacement tests, suggesting that there was a wide variability in weld reliability.



Component and System Level Simulations Can Not Afford all of the Details of Welds



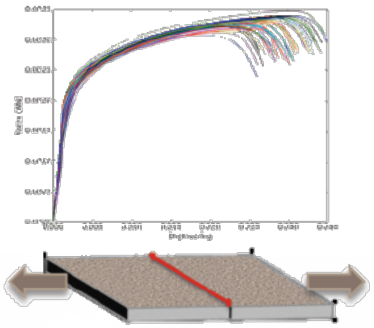




Frank Dempsey, Amalia Black → Jill Suo-Antilla → Charlie Robino

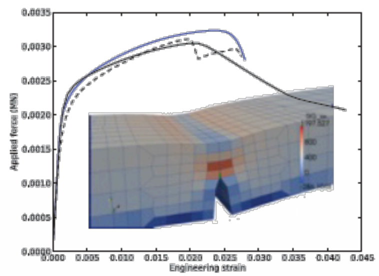
"Homogenization" is the process by which detailed behavior at a lower length scale is simplified so that it can be captured at a higher length scale *without loss of realism*.

Stochastic Reduced Order Modeling (SROM) provides an optimum pathway to upscale knowledge of statistical uncertainties to component & system-level performance predictions



experiments for 304-L laser welds

Σ



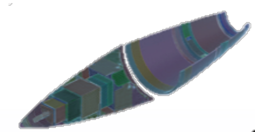
calibration of constitutive parameters

$c(\boldsymbol{\sigma}_i) = \boldsymbol{e}_i$

$\mathrm{SROM}(\boldsymbol{E}) \mapsto \tilde{\boldsymbol{E}}$

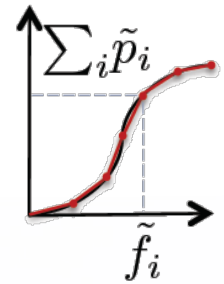
$\{\tilde{\boldsymbol{e}}_i, \tilde{\boldsymbol{p}}_i\}$

stochastic reduced order model

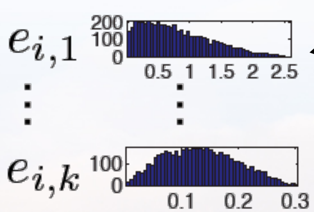


$s(\boldsymbol{u}; \tilde{\boldsymbol{e}}_i) = \tilde{f}_i$

surrogate model



probability of failure



E

Statistical distributions of inhomogeneities are optimally subsampled (“smart Monte Carlo”)

-Geometric variations in weld depth
-Variations in porosity
-Variations in microstructure
-etc.

Corporate Level 2 Milestone

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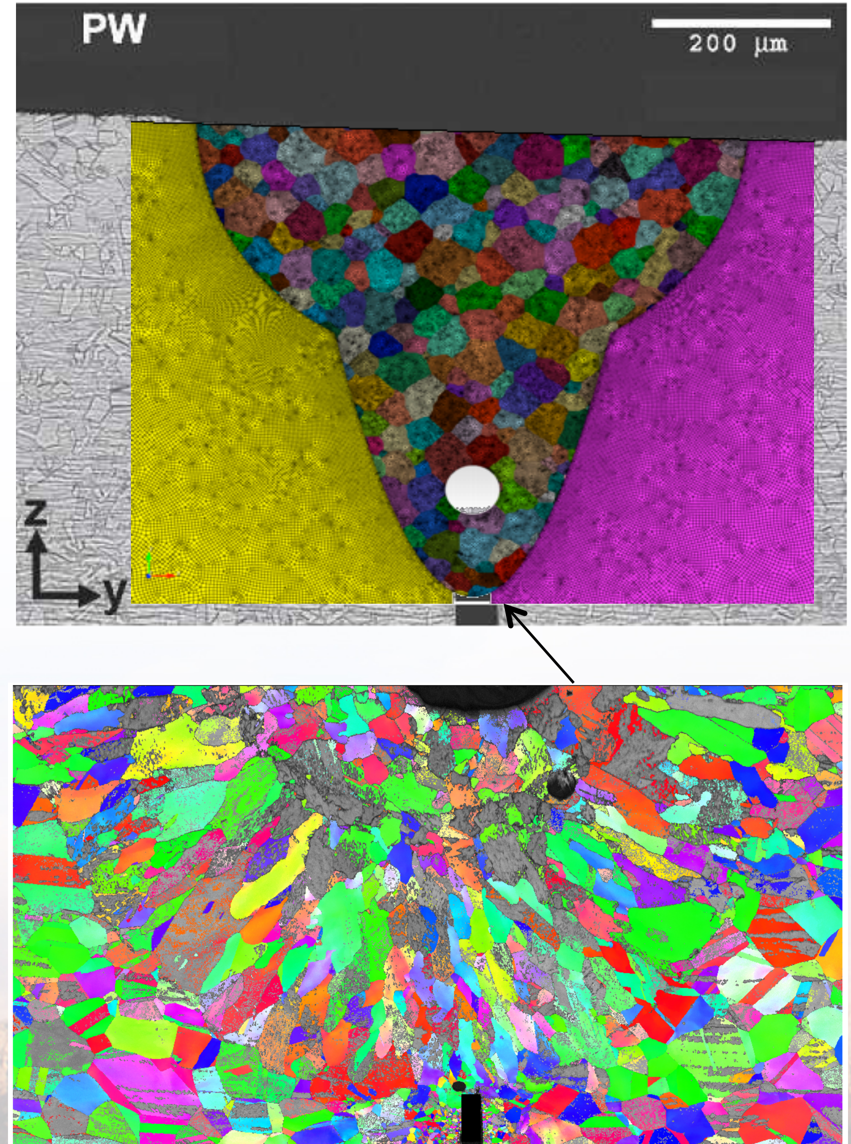
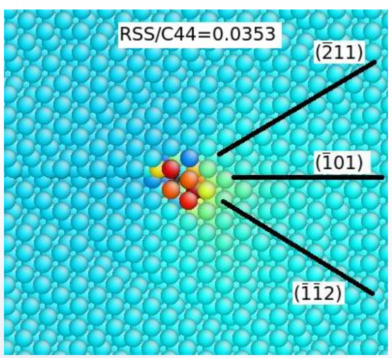
Porosity in laser welds provides one illustration of the PPM goal of understanding material variability in structural metals



Crystal Plasticity Modeling discretely models each grain in the material with its elastic and plastic anisotropy.

- **Crystal plasticity =** Grain-level (mesoscale) approach **to materials modeling using multiscale strategies**
- **Explicitly model** discrete **grains and slip systems (anisotropy, texture evolution,…)**

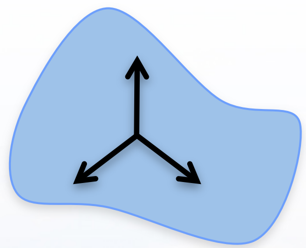
Atomic phenomenology: Fundamental deformation mechanisms



Yield criterion

$$\sigma_{cr}^{app}[a_0 \mathbf{m}^{(s)}\mathbf{n}^{(s)} + a_1 \mathbf{m}^{(s)}\mathbf{n}^{(s')} + a_2\left(\mathbf{n}^{(s)} \times \mathbf{m}^{(s)}\right)\mathbf{n}^{(s)} + a_3\left(\mathbf{n}^{(s)} \times \mathbf{m}^{(s)}\right)\mathbf{n}^{(s')}] = \tau_{cr}$$

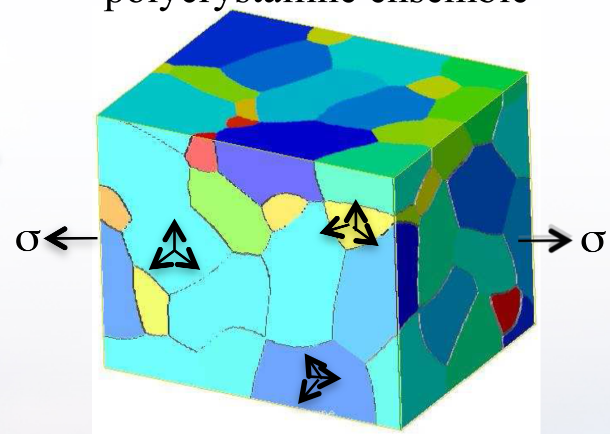
Single crystal plasticity: Deformation of one, isolated crystal



Constitutive law

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

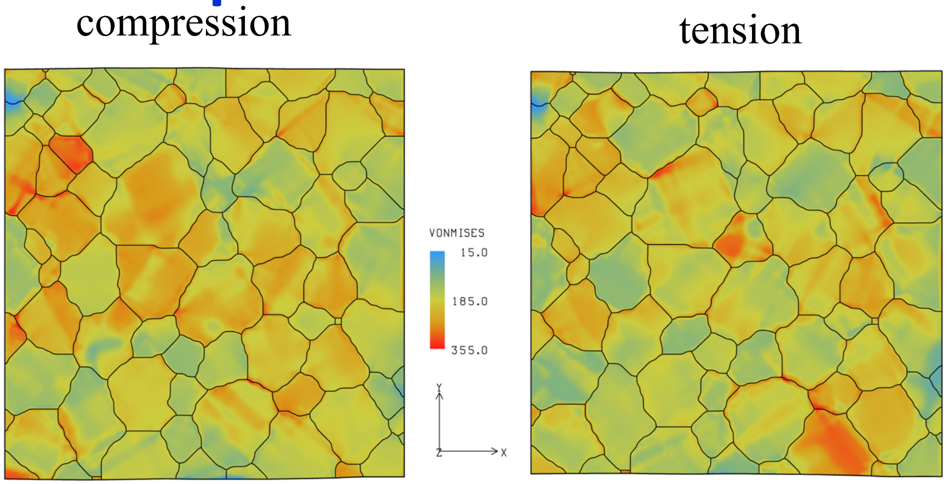
Polycrystal plasticity: Assemble single crystals into polycrystalline ensemble

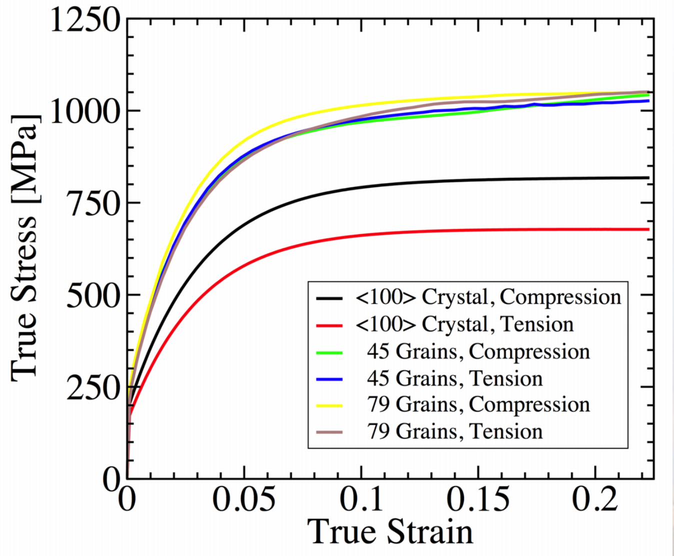


Prediction of collective deformation behavior

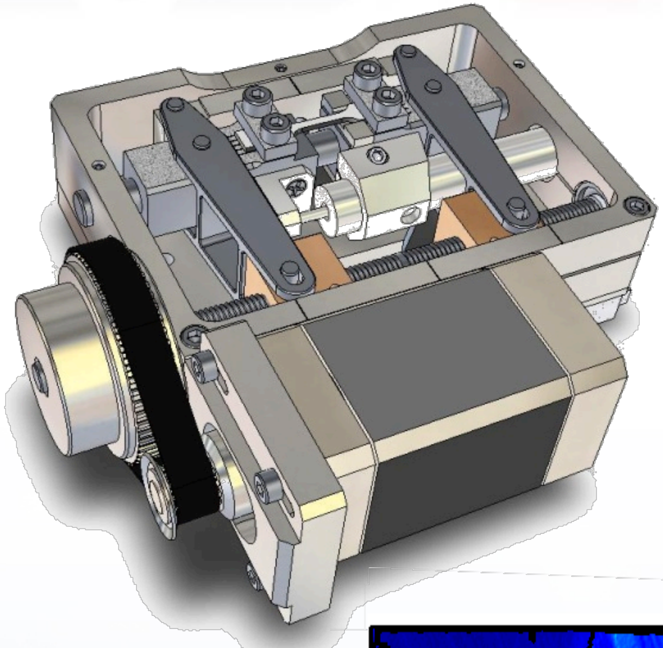
Crystal plasticity predicts the inhomogeneous partitioning of stress and strain within the material, and the resulting macroscopic stress-strain behavior

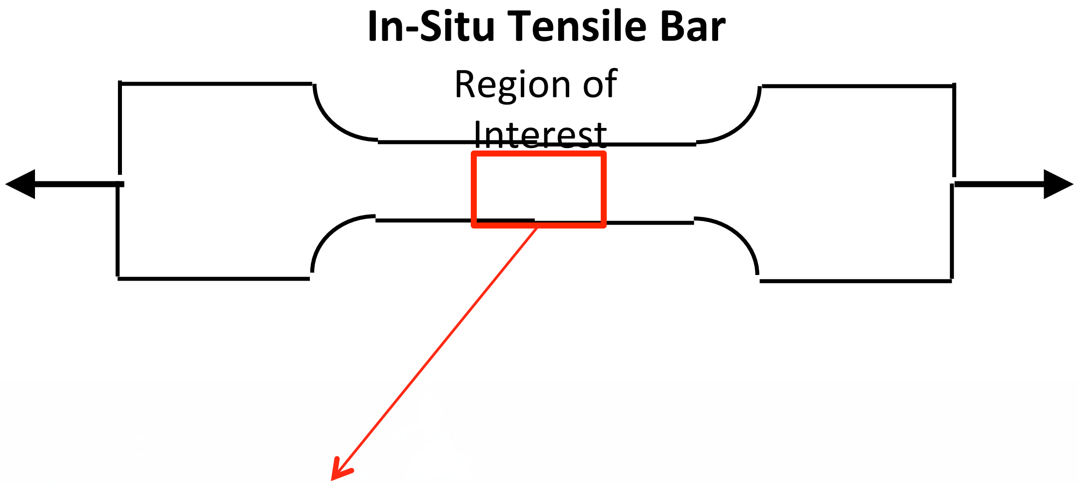
- **Microstructural simulations give continuum behavior:**
  - Stress-strain curves show how material properties vary with microstructure.
- **Microstructural simulations also give local behavior:**
  - The local stress distribution shows how critical features vary with grain structure and stress state.
- ***Microstructural simulations quantify local and global variability in material properties.***

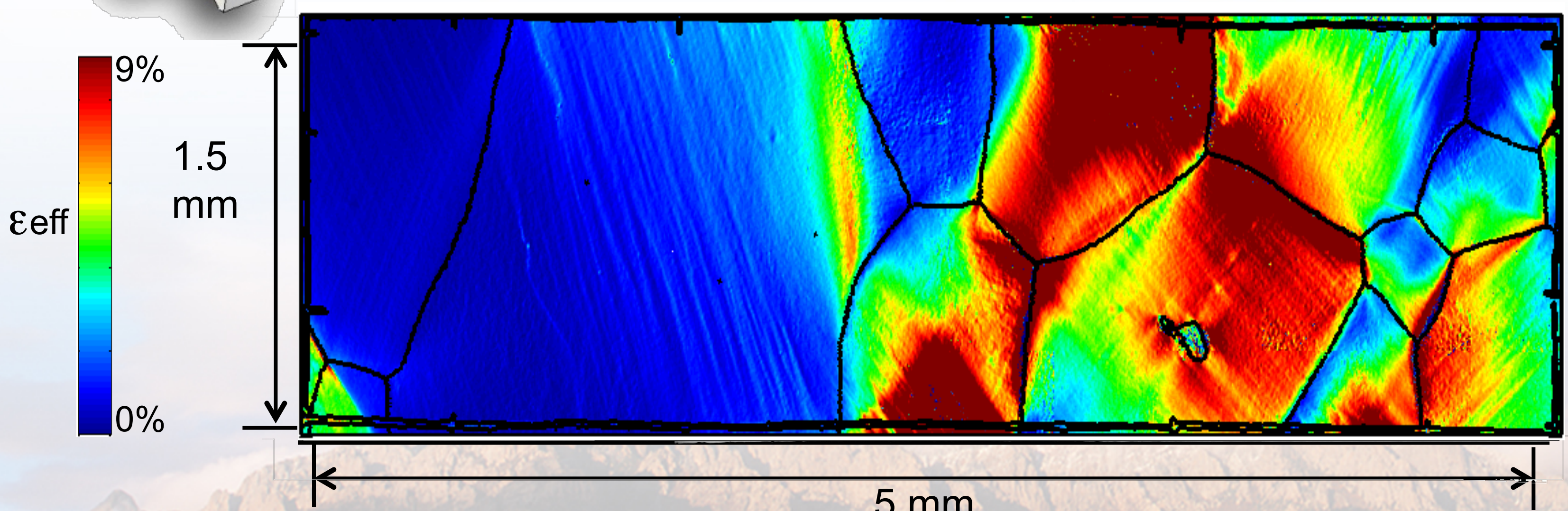




In-Situ SEM loadframe allows direct observation of local deformation





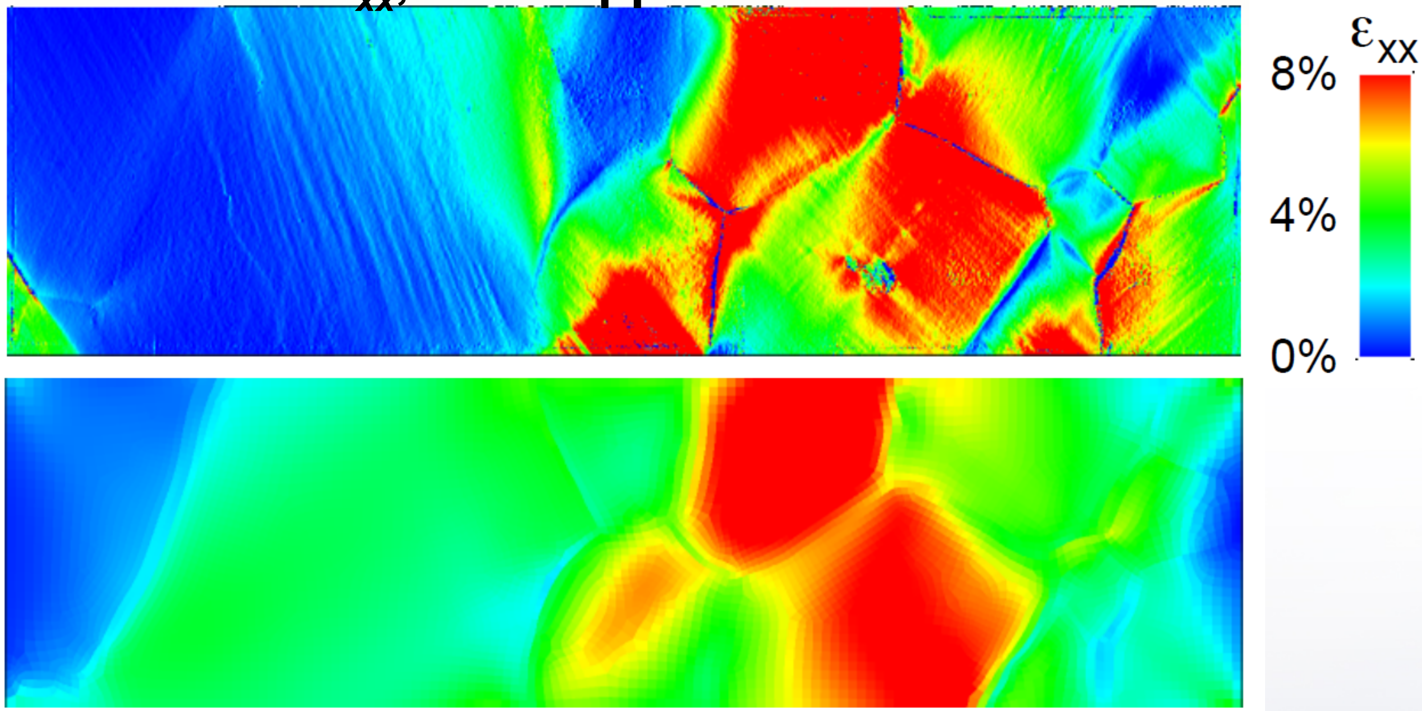


Early comparison of strain from experiments and models is promising.

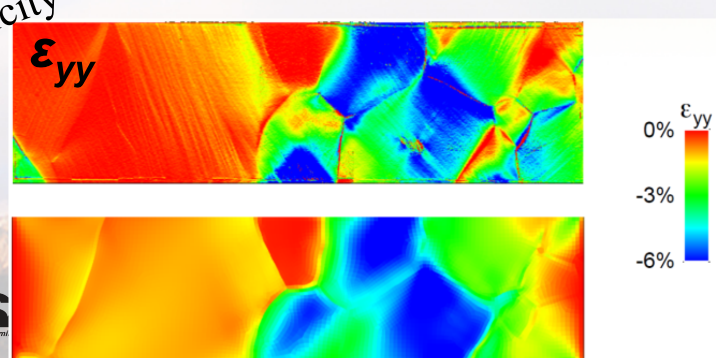
ε_{xx}, 4.2% Applied Strain

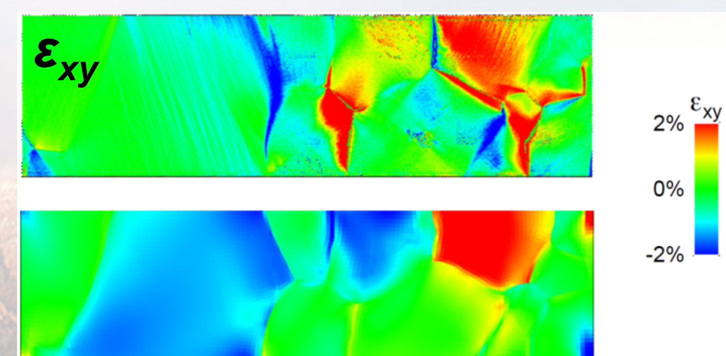
DIC Measurements
(Digital Image Correlation)

CP-FEM Simulation
(Crystal Plasticity Finite Element Method)



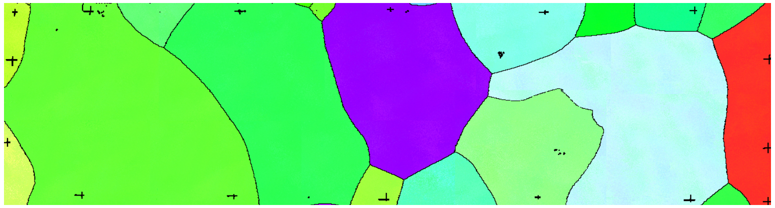
Keynote Presentation At 2013 International Symposium on Plasticity



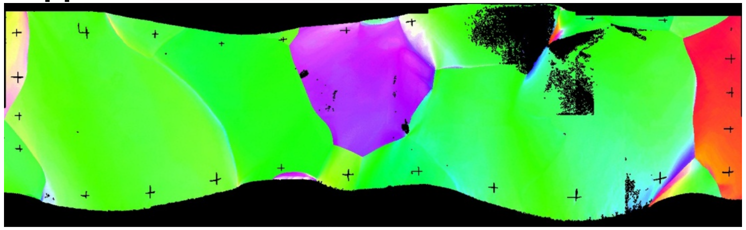


Model also predicts how grains rotate to accommodate deformation

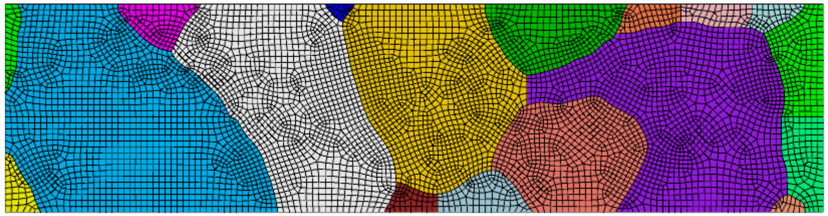
EBSD Before Deformation



ε_{appl} = 19%

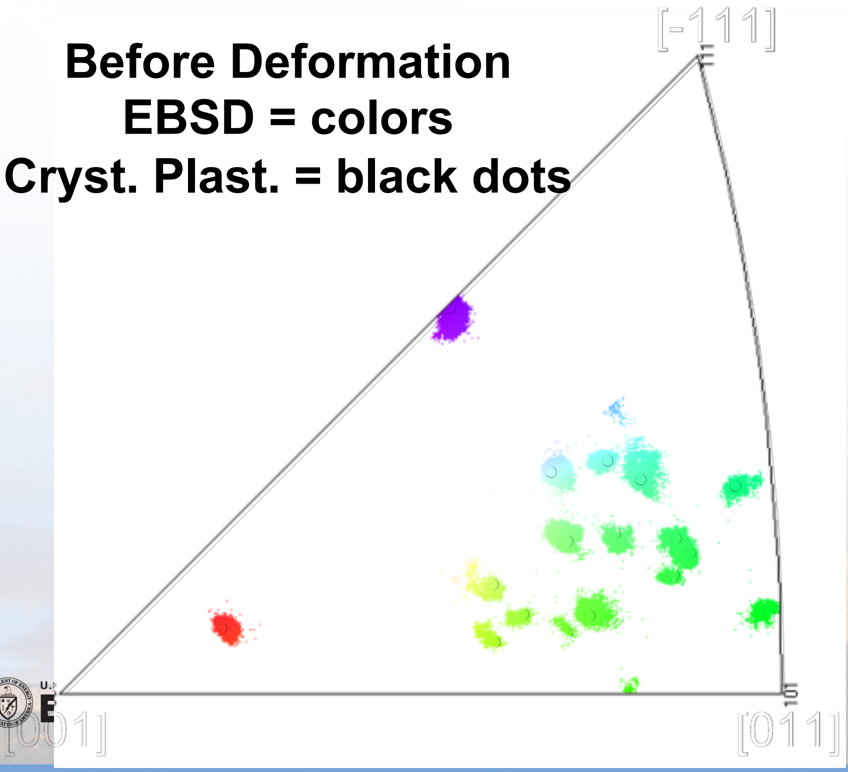


Splined Grain Boundaries →

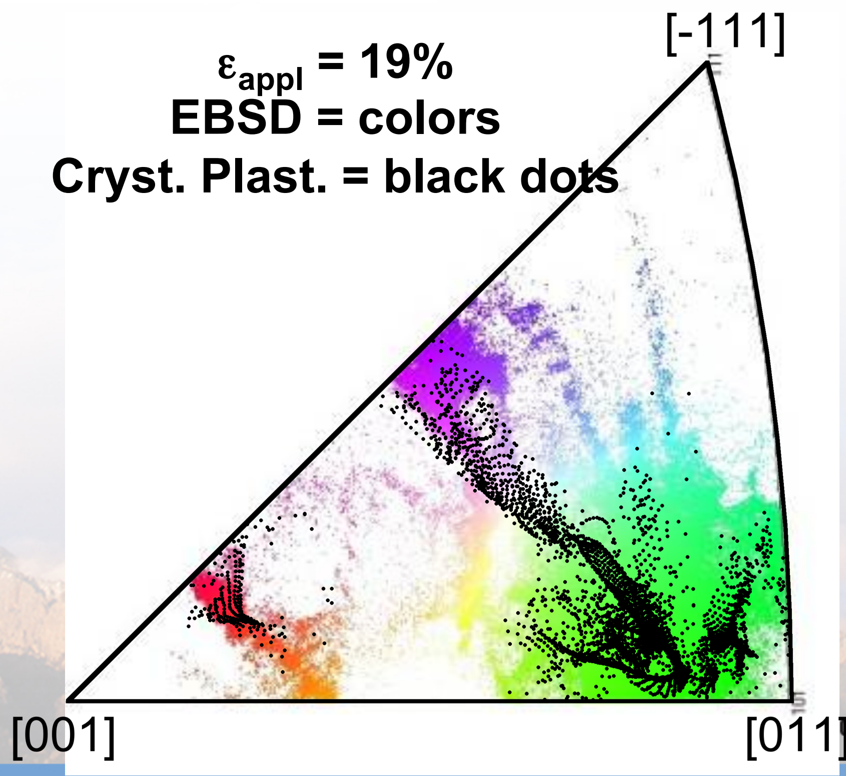


← **One Orientation per Grain**

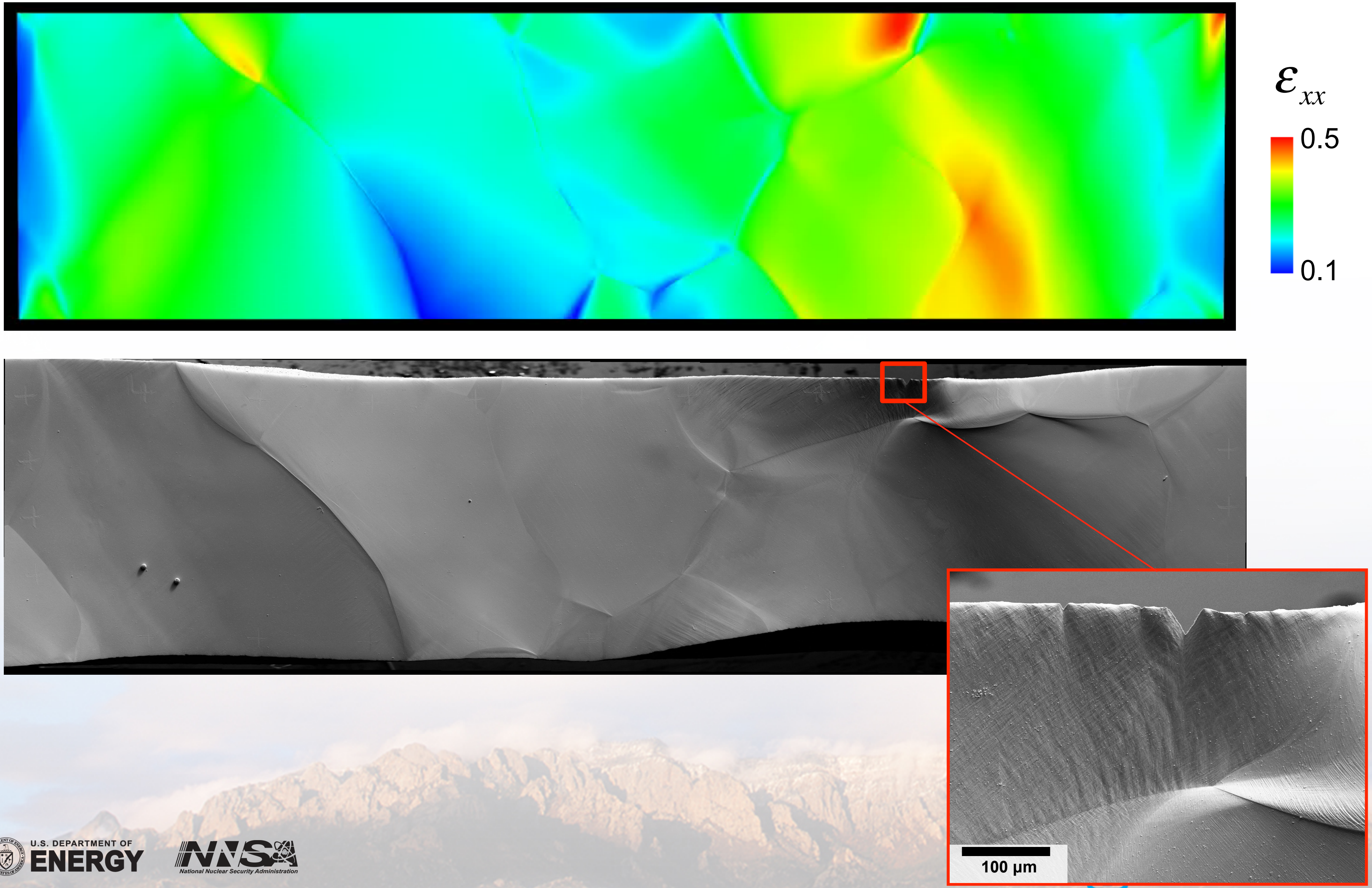
Before Deformation
EBSD = colors
Cryst. Plast. = black dots



ε_{appl} = 19%
EBSD = colors
Cryst. Plast. = black dots



Can our crystal plasticity model predict the influence of microstructure on failure?



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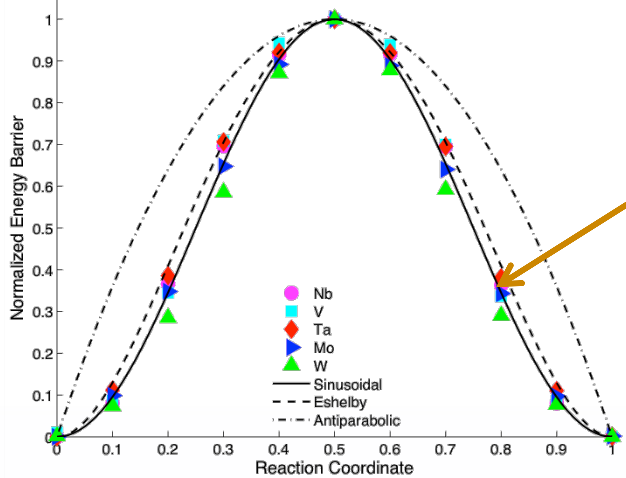
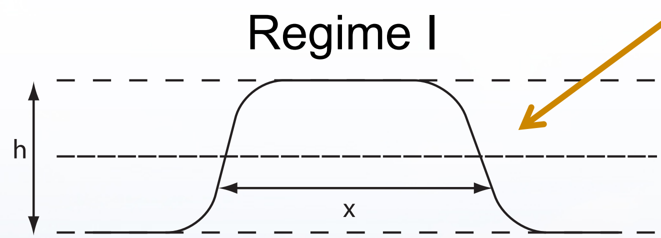
The success of crystal plasticity ties back to detailed atomistic-level understanding of dislocation processes



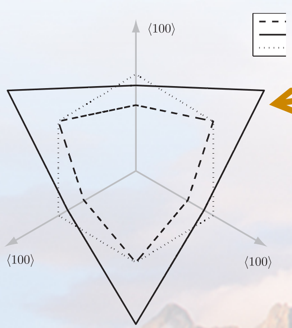
- Determine the Shape of the Peierls Potential from atomistics/DFT.

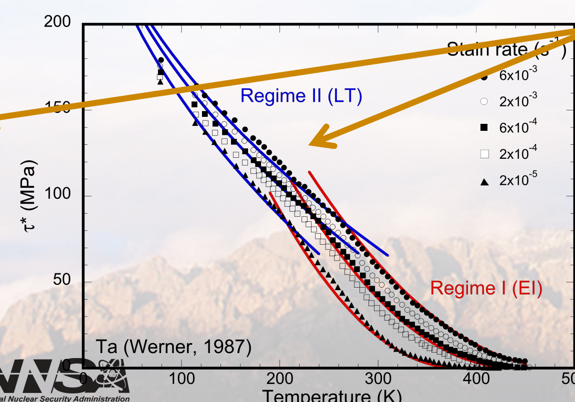


- Use atomistics to inform continuum models of the Peierls potential and it stress dependence.

$$\dot{\gamma} = \dot{\gamma}_o \exp\left(\frac{-\Delta G^*}{k_B T}\right) \quad \Delta G^*_{kp} = 2G_k - \left(\tau \mathcal{E} b h^3/2\right)^{1/2}$$

$$\tau = \tau_o \left(1 - \frac{T}{T_k}\right)^2$$





- Use continuum models to build single crystal yield laws that are temperatures, strain rate, and stress dependent.

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Where is PPM heading…

- Adding strain-rate laws to extend to dynamic / shock loading conditions
- Extending from room temperature to high-temperature behavior
- Adding details of grain boundary hardening
- Moving from single-phase materials to multi-phase materials
- Maturing and validating statistical homogenization schemes
- Develop a robust microstructural-scale failure criterion
- Adding process-awareness to understand effects of process changes on reliability.

We are in the process of planning the next 3 years of PPM to maximize its positive impact on NW through building needed materials science expertise and capabilities.

Summary

- PPM continues to build momentum, thanks to the support from S&T management (ASC, RTBF, ESC).
- The core focus of mechanical reliability of structural metals is a theme that connects to numerous components.
- PPM is building the computational and experimental infrastructure to tie basic science of metal deformation and fracture from the atomistic scale up to component scale.