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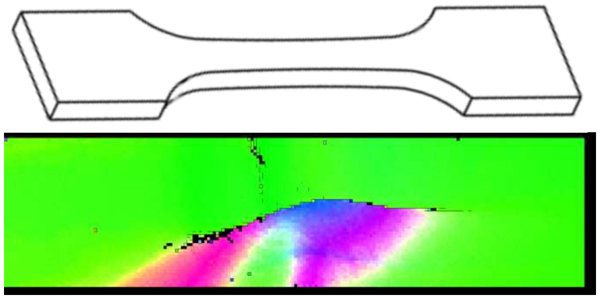
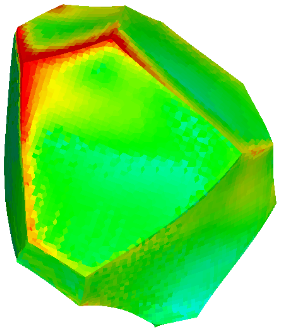
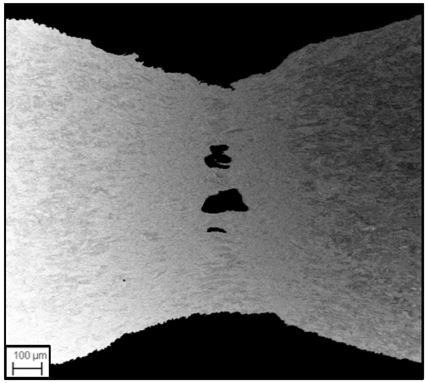
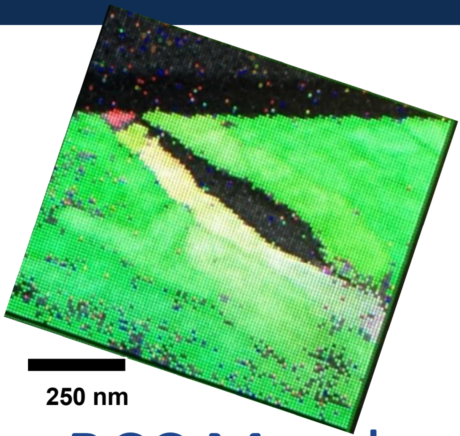








Ductile Void Nucleation in Pure BCC Metals under Quasi-static Loading

Brad Boyce, Blythe Clark, Jay Carroll, Philip Noell, Ryan Sills
Materials Science and Engineering Center
Sandia National Laboratories

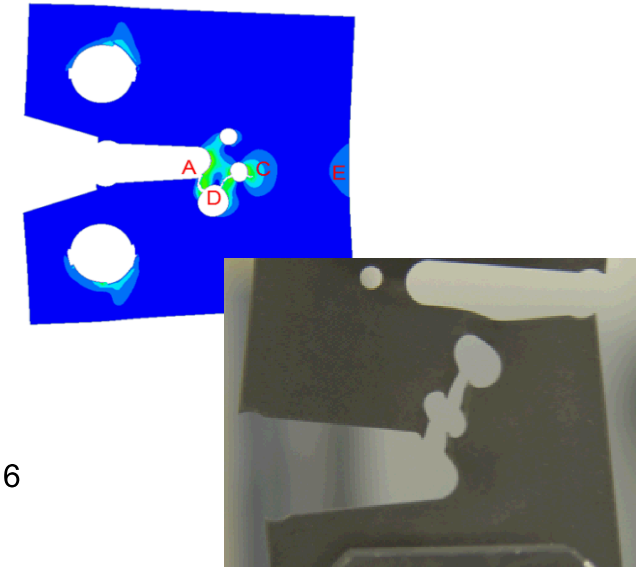
June, 2017

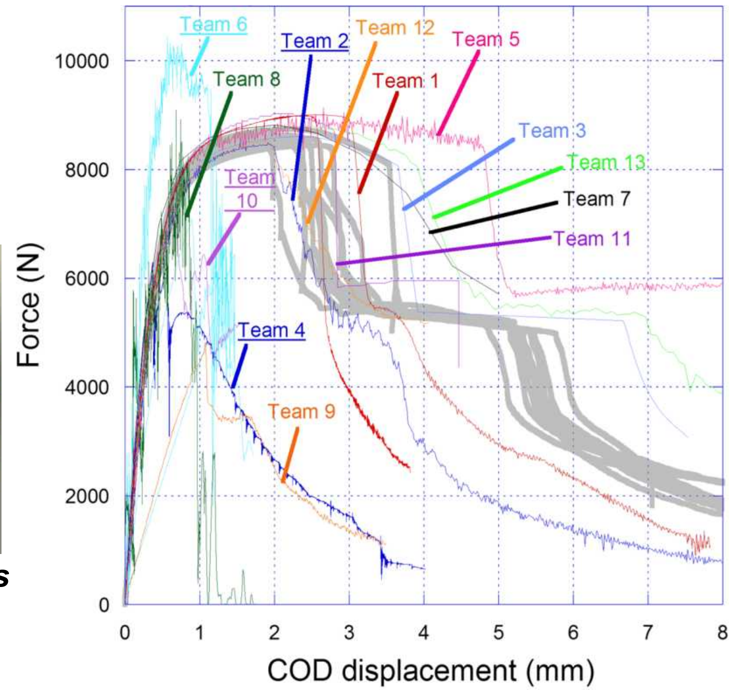
Int. Conf. on Fracture

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

The Sandia Fracture Challenge explores the limits of ductile failure prediction

Special Issues in 2014 & 2016





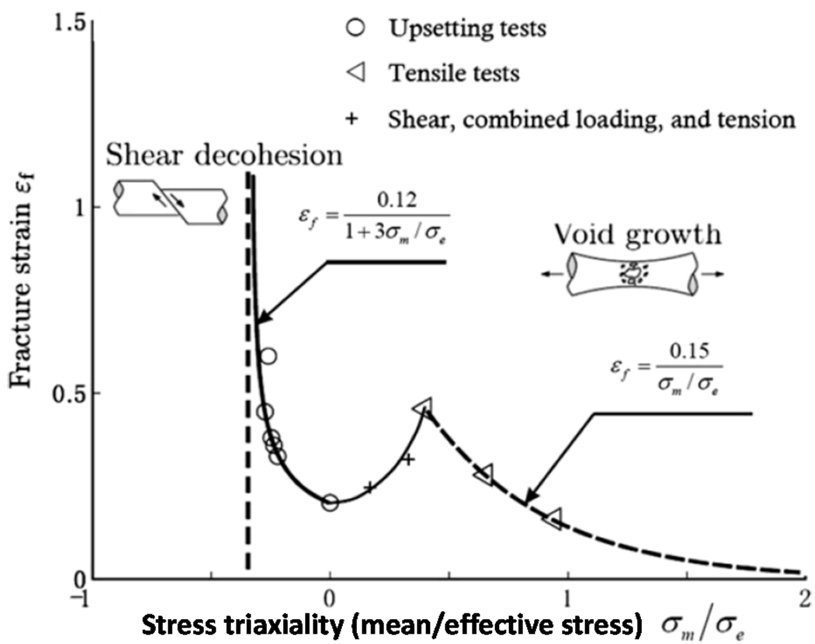
We have built an ***International Consortium of >30 volunteer organizations***

- Lack of consensus on the governing equation for void rupture
- Deterministic methods struggle with microstructurally rare events
- State of the art involves empirical continuum models

Models for void nucleation are largely empirical

$$\dot{\phi} = \sqrt{\frac{2}{3}}\dot{\epsilon}_p \frac{1-(1-\phi)^{m+1}}{(1-\phi)^m}\cdot \sinh\left[\frac{2(2m-1)}{2m+1}\frac{\langle p\rangle}{\sigma_e}\right] + (1-\phi)^2\,\dot{\eta} v_{vo}.$$

Void growth | Void nucleation



Nahshon and Hutchinson, Europ. J. Mechanics A, 2008

Additional nucleation models

Gurland and Plateau, 1963
Ashby, 1966
Coleman and Gurtin, 1967
Rosenfield, 1968
Barbee et al., 1972
Argon et al., 1975
Raj and Ashby, 1975
Gurson, 1977a, b
Needleman and Rice, 1978
Goods and Brown, 1979
Tvergaarrd, 1982a
Saje et al, 1982
Hirth and Nix, 1985

Void nucleation rate — Fitting parameters

$$\dot{\eta} = \eta\dot{\epsilon}_p\left\{N_1\left[\frac{4}{27}-\frac{J_3^2}{J_2^3}\right] + N_2\frac{J_3}{J_2^{3/2}} + N_3\left\|\frac{I_1}{\sqrt{J_2}}\right\|\right\}N_4$$

void content — strain-rate — stress state descriptors

Horstemeyer and Gokhale, *Int. J. Solids. Struct.*, 1999

Vacancy Condensation

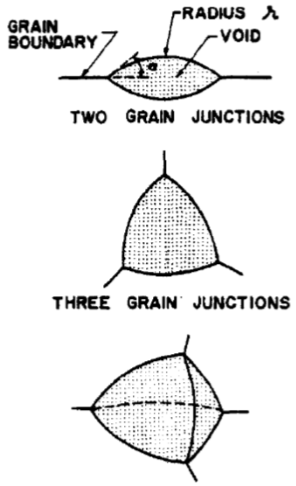
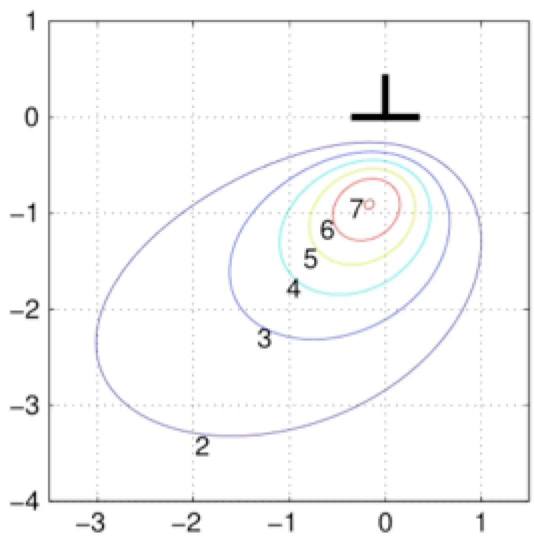


Fig. 1. Void geometries in inclusion free grain boundaries.

Raj and Ashby, Acta Metallurgica, 1975



Sills and Cai, Phil. Mag, 2016

Voids are thought thought to form by vacancy condensation at **grain boundaries** (Raj and Ashby, 1975)

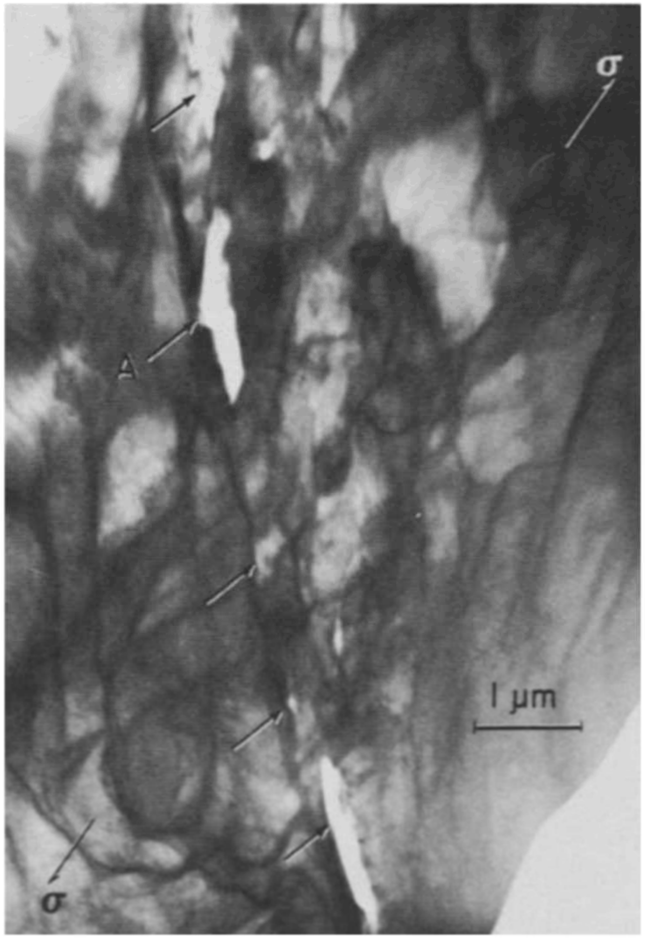
At lower temperature, is thought to require high hydrostatic tensile stress (inherently difficult to observe at free surfaces)

When vacancy sources and sinks are present, requisite stress is substantially lower (Hirth and Nix 1985).

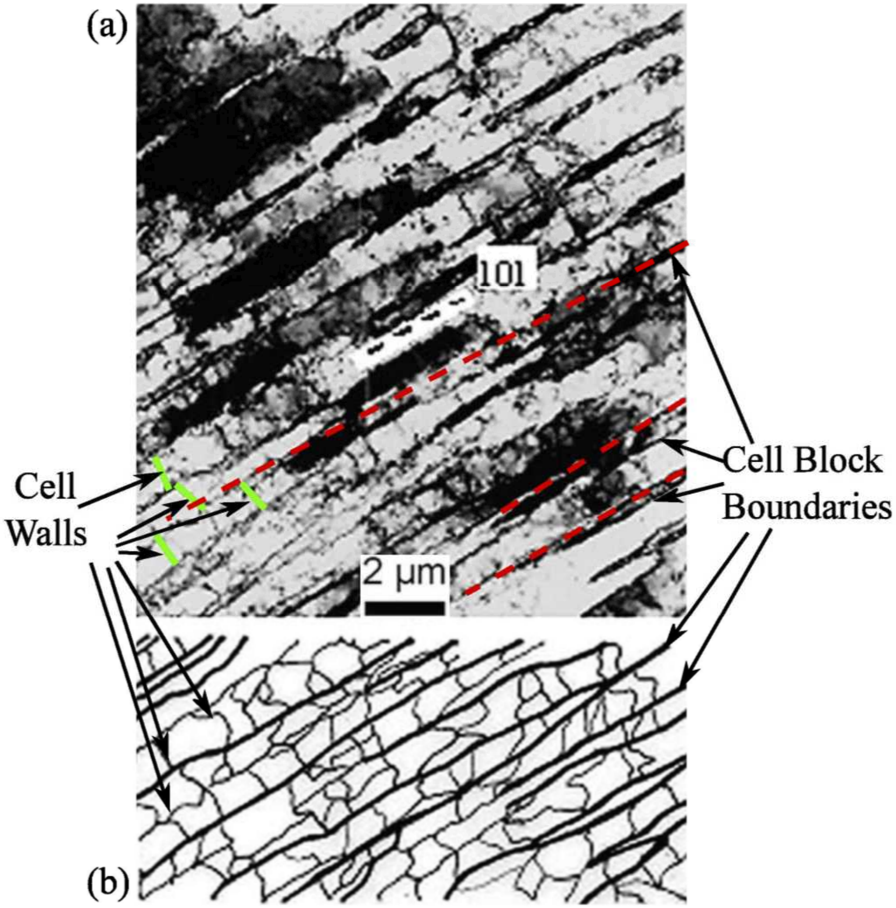
Dislocation climb is a potential vacancy source at high temperatures

Gliding dislocations drag solute, and by extension vacancies (Sills and Cai, Phil Mag, 2016)

Tools and Understanding of Microstructure have improved over the past 30+ years



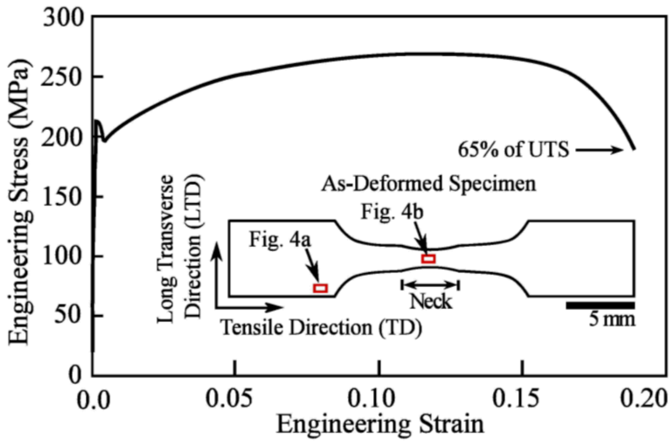
R. N. Gardner, T. C. Pollock, and H. Wilsdorf, "Crack initiation at dislocation cell boundaries in the ductile fracture of metals," *Materials Science and Engineering,* vol. 29, no. 2, pp. 169-174, 1977.

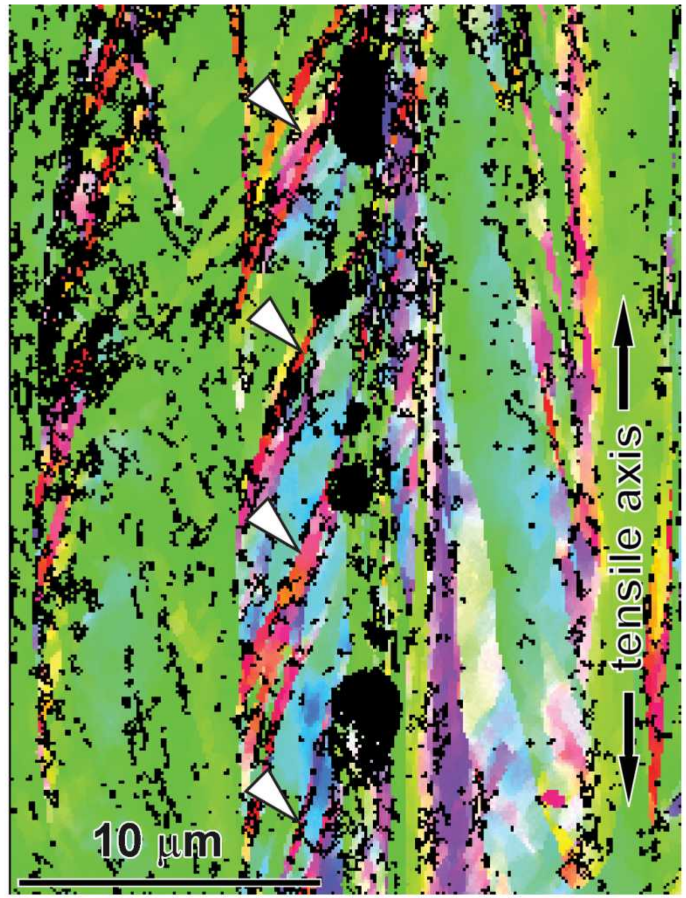


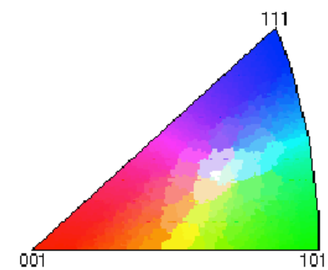
B. Li, A. Godfrey, Q. Meng, Q. Liu, and N. Hansen, "Microstructural evolution of if-steel during cold rolling," *Acta Materialia,* vol. 52, no. 4, pp. 1069-1081, 2004.

Initial Observation…

Interrupted tension +
Cross-sectional metallography
+ EBSD





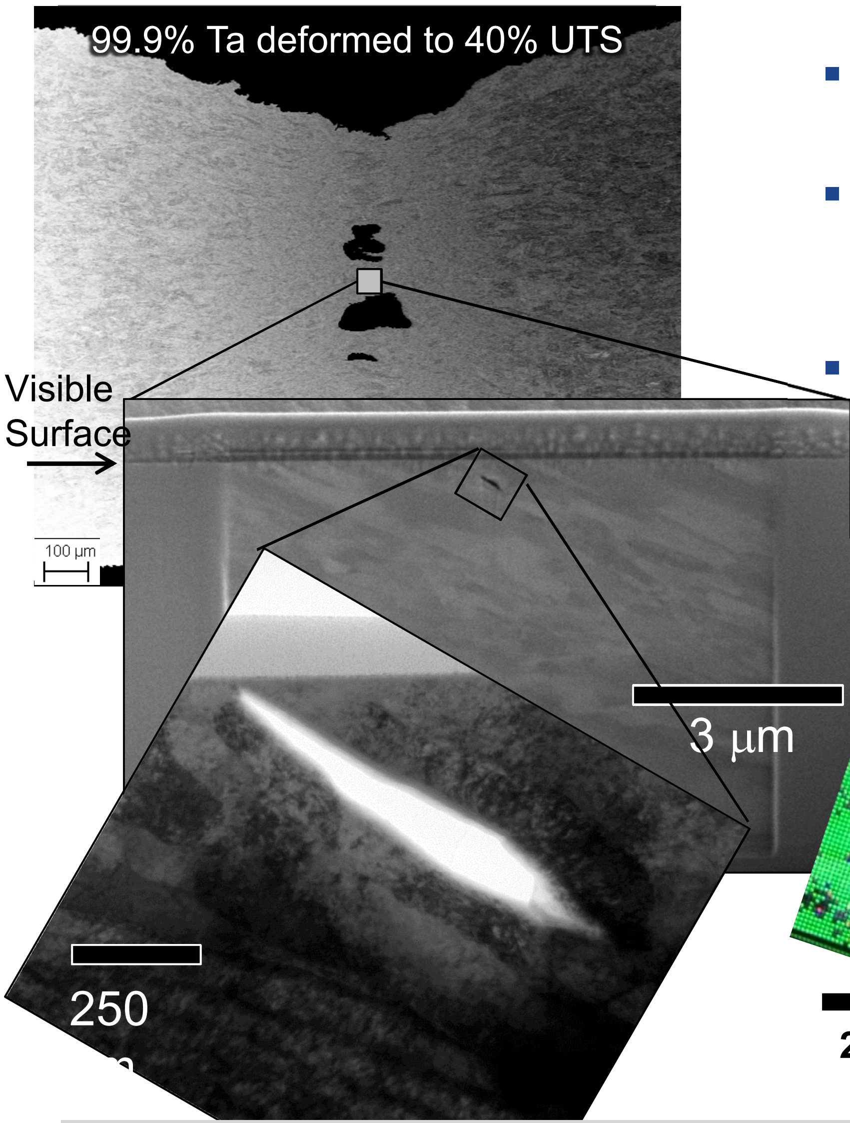


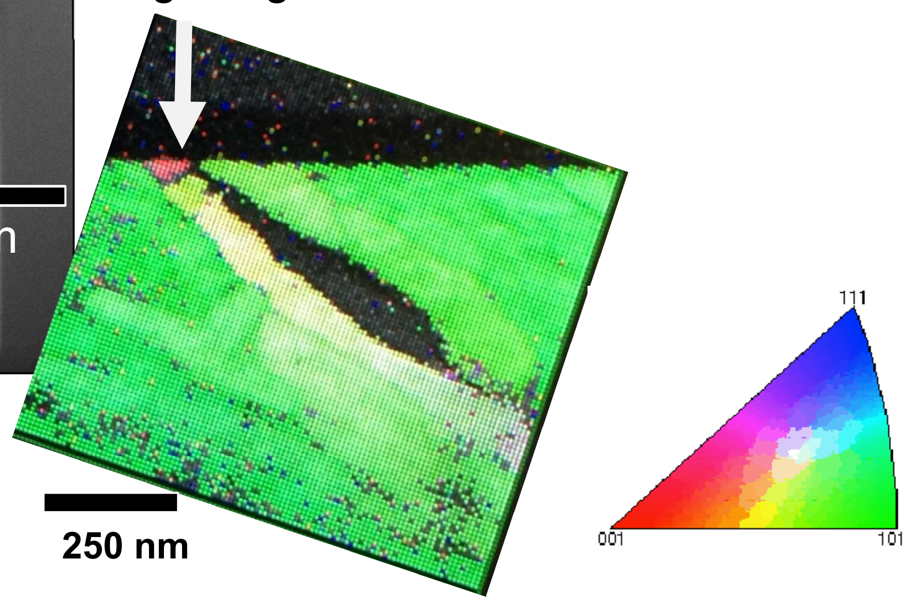
From Boyce et al., *Metall. Mater. Trans. A*, 2013

Hypothesis: void nucleation under tension in pure metals occurs when the dislocation network forms intense cell walls that are detected as high-angle subgrain boundaries.

"Treasure Hunt"

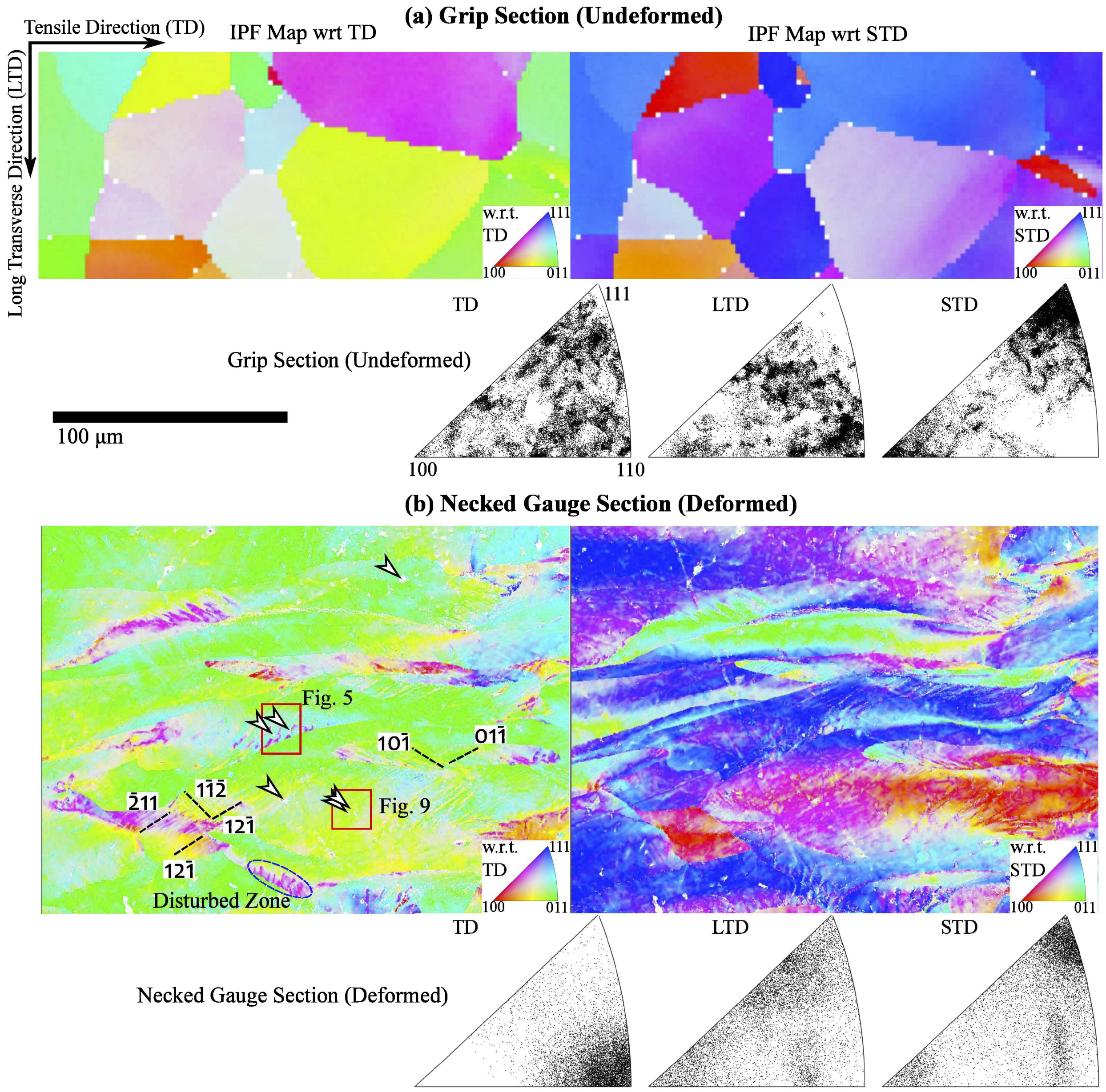
- Focused Ion Beam (FIB) used to locate subsurface, deformation-induced voids in interrupted tensile bar.
- Void shape is aligned with subgrain boundaries.
- Transmission Kikuchi Diffraction (TKD) to determine crystallographic orientation near void.
- Orientations are consistent with EBSD analysis showing void nucleation along high angle misorientation boundaries



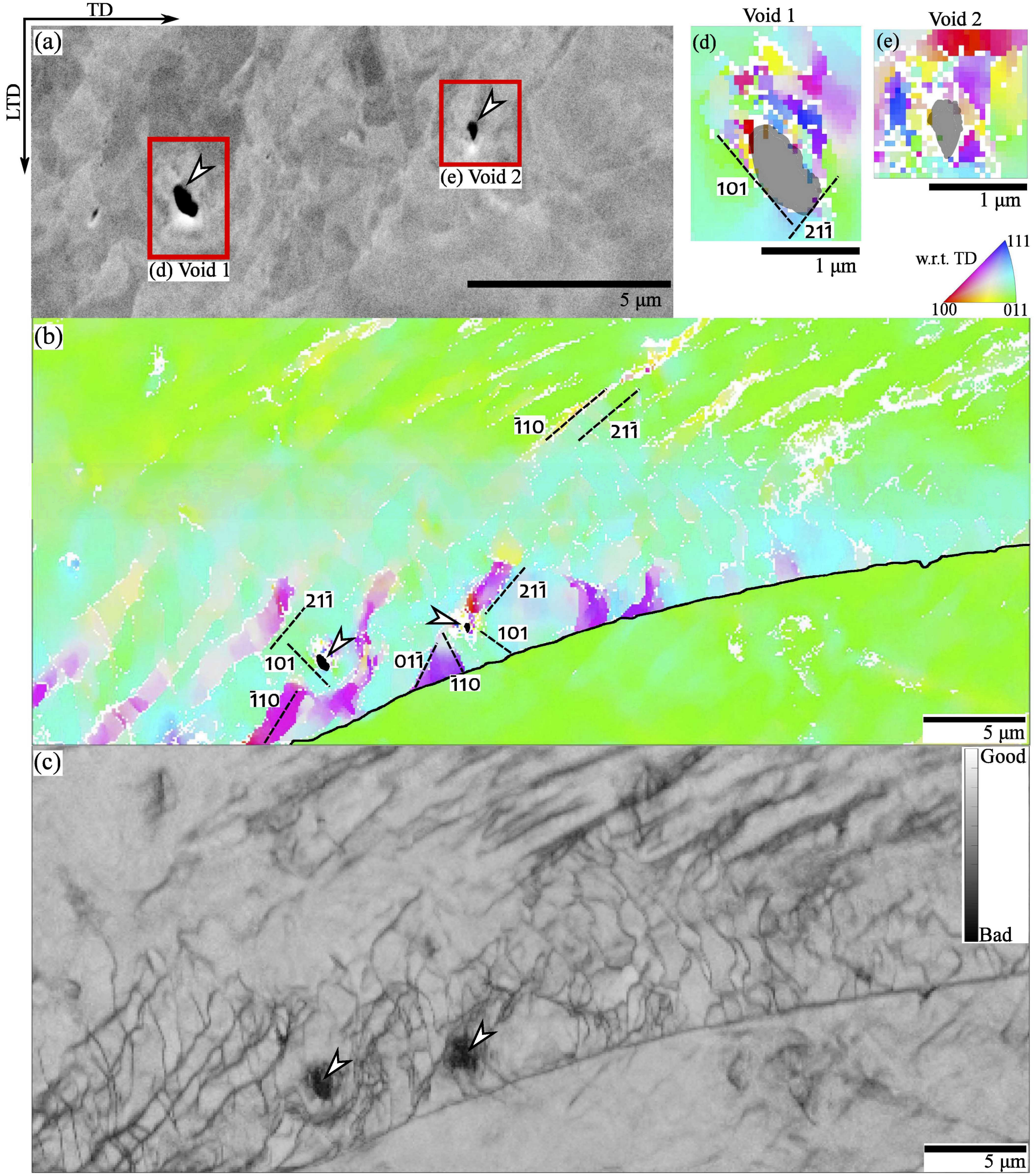


Hypothesis: void nucleation under tension in pure metals occurs when the dislocation network forms intense cell walls that are detected as high-angle subgrain boundaries.

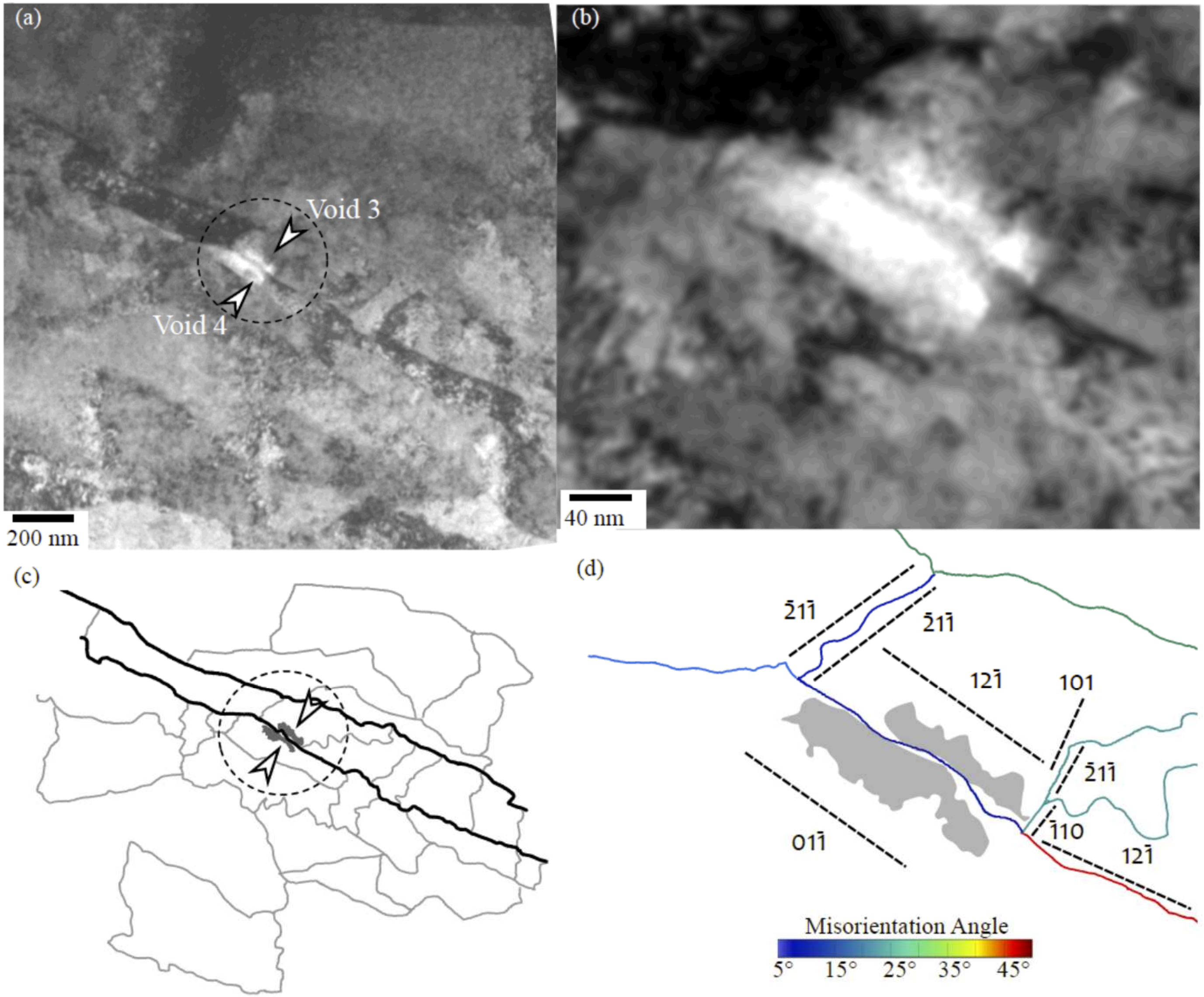
Overview of Highly Deformed Necking Region…



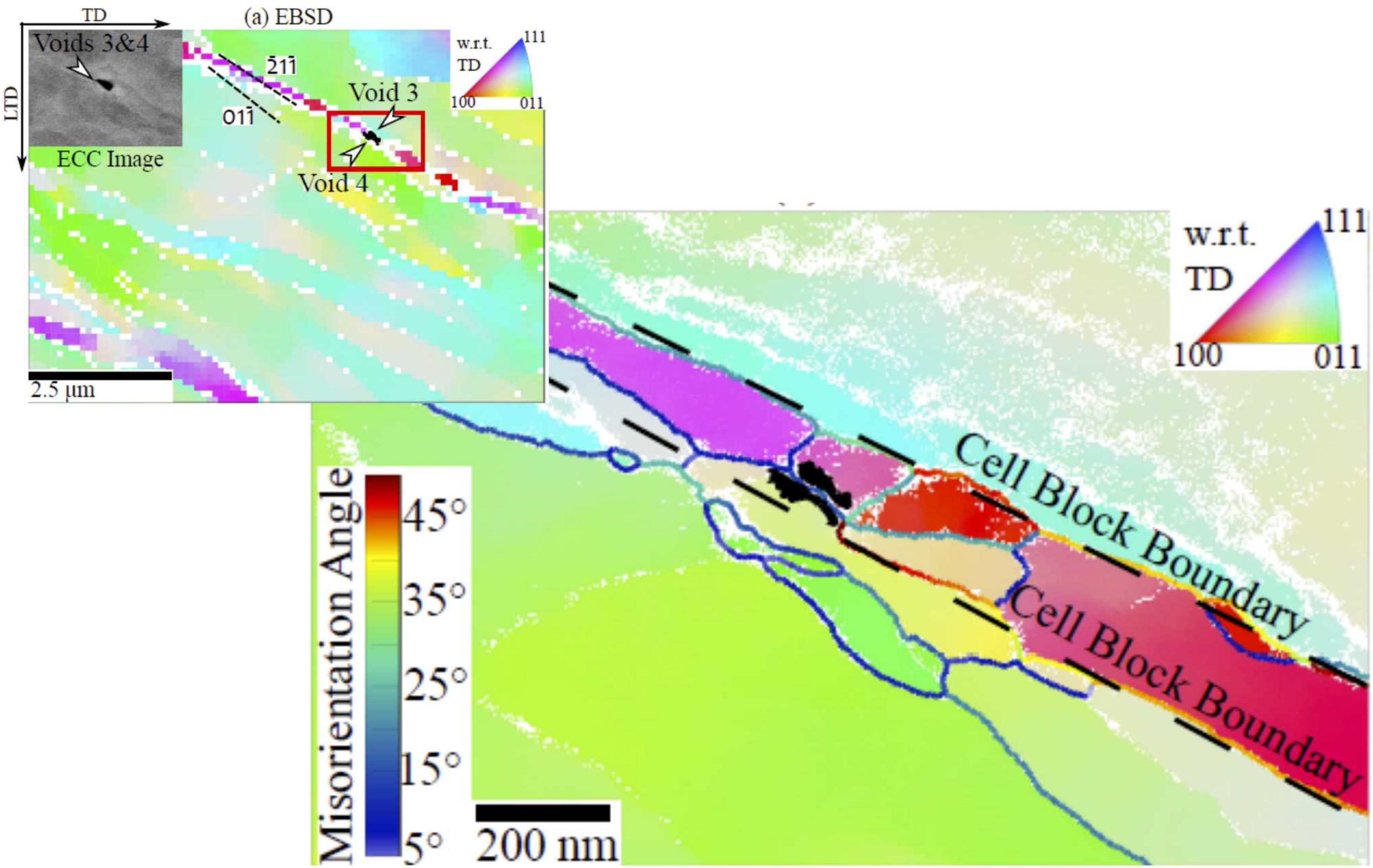
Voids 1 and 2 at Cell Block Boundaries near a GB



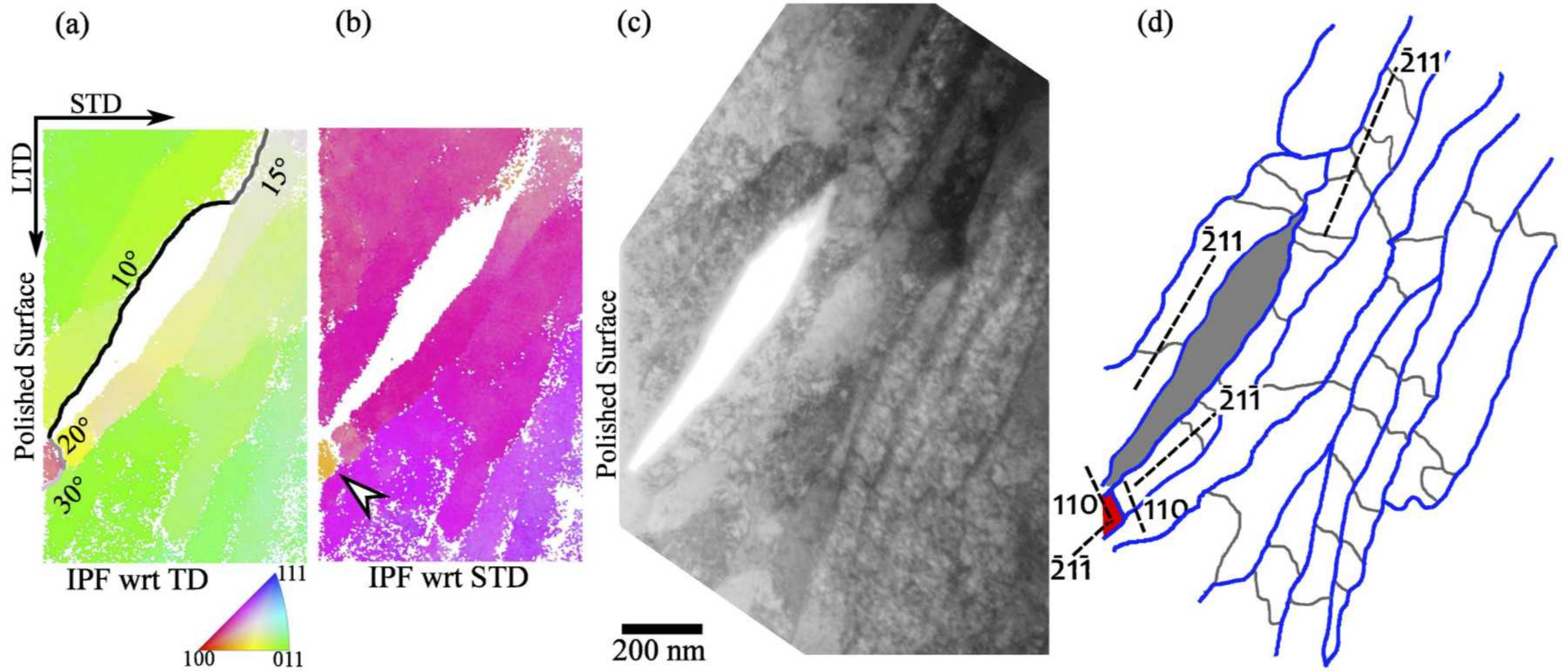
Voids 3 and 4 at a Cell Block Boundary "Isthmus"



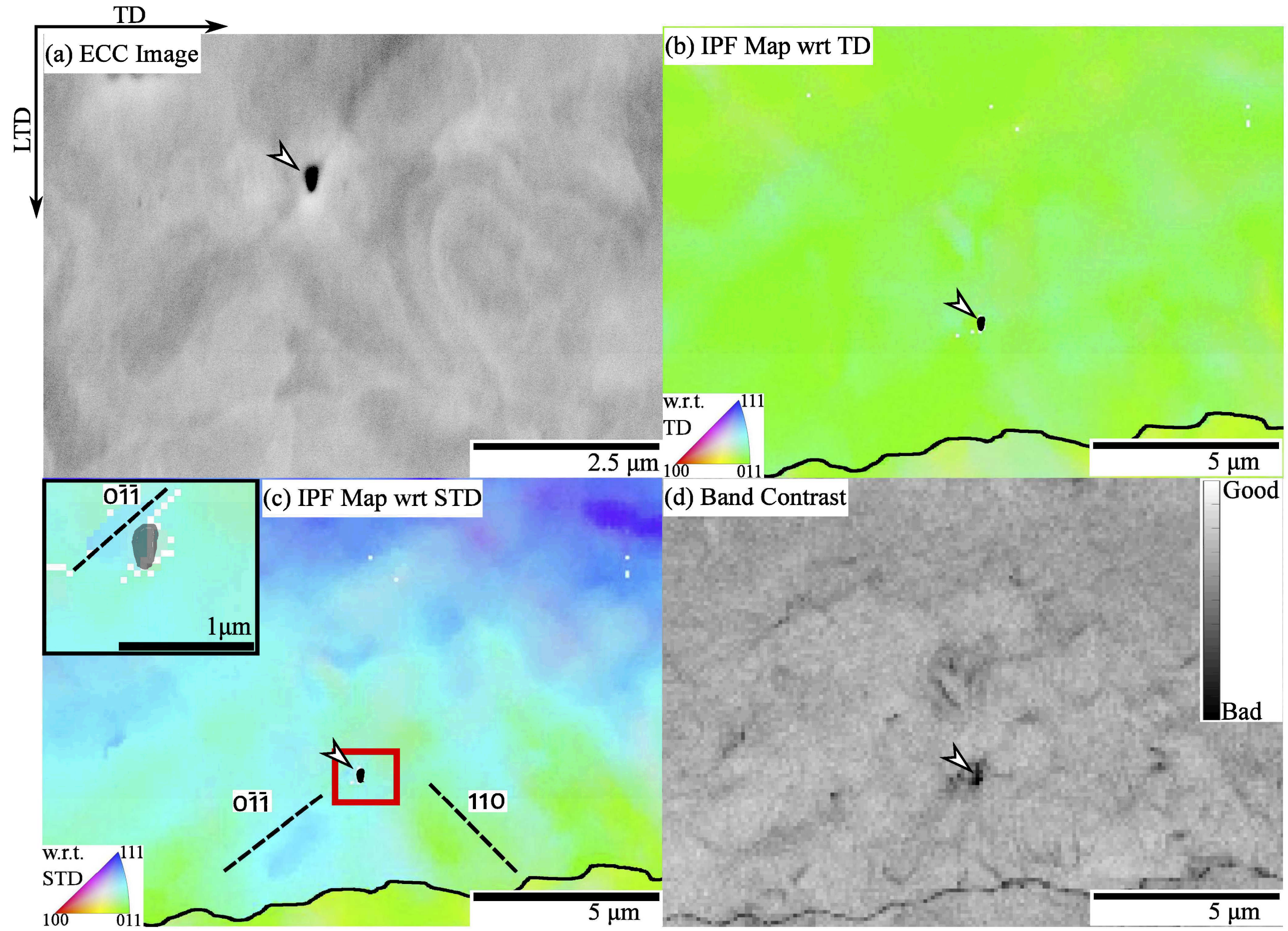
Voids 3 and 4 at a Cell Block Boundary "Isthmus"



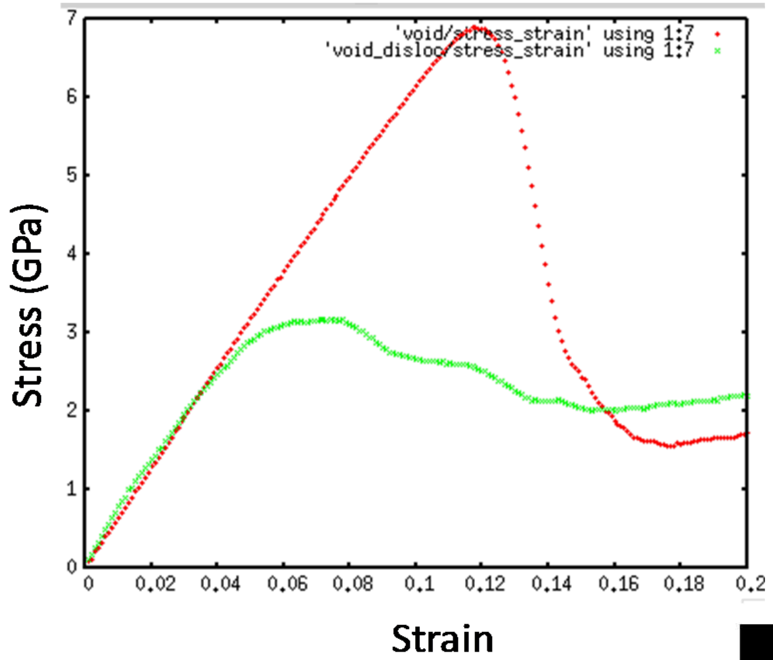
Revisiting the "Treasure Hunt" Void



A few voids (2 of 20) did not seem to involve misorientation boundaries due to lack of subsurface (3D) data?



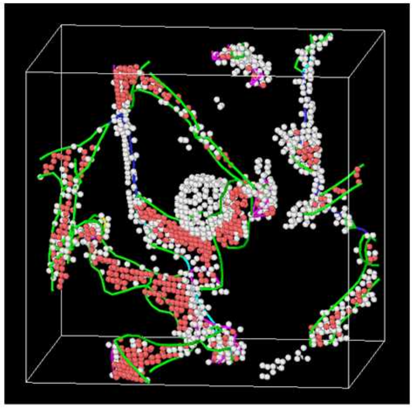
Modeling Void Nucleation & Growth



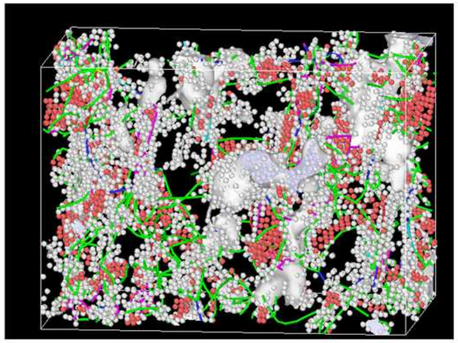
- The classical theory for deformation-induced void growth is that voids grow by dislocation emission.
- Our work and others [Bringa et al, 2010] have shown that void growth by dislocation emission requires very large stresses ~7 GPa

We hypothesize that voids grow by dislocation consumption

- Molecular Dynamics simulations are underway to assess the dislocation consumption hypothesis
- Experiments underway to assess the dislocation substructure in the vicinity of voids.



initial
Dislocation density: 1.1e17 m^{-2}



20% strain
Dislocation density: 4.1e17 m^{-2}

Summary…

Under quasi-static loading, pure Ta forms incipient voids primarily at cell block wall boundaries.

Nucleation is often associated with an extensive local misorientation network

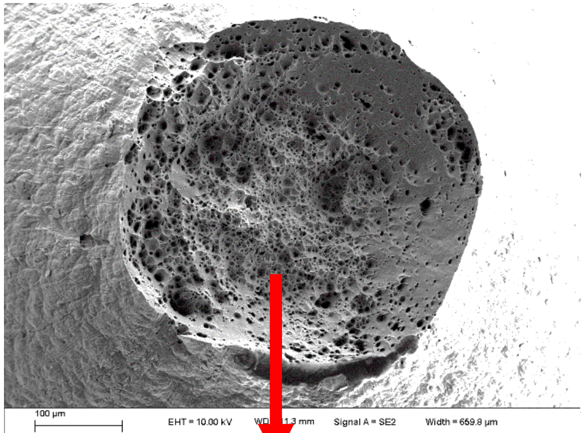
These highly deformed zones are often in the grain “mantle”, near but not at grain boundaries

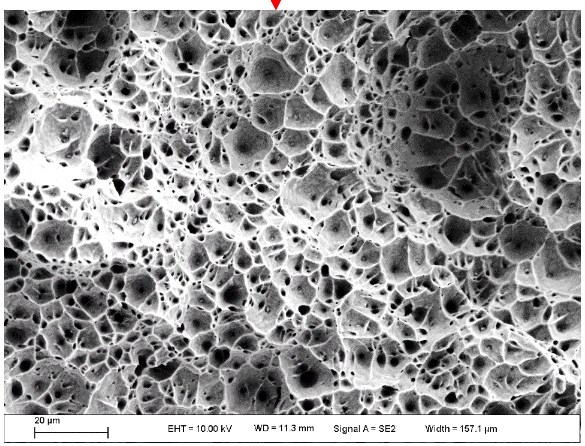
Direct modeling by dislocation dynamics, crystal plasticity, or macroscale finite element would be difficult.

Molecular dynamics models suggest that certain dislocations impinging on Voids serve to facilitate growth…

Void morphology strongly depends on purity

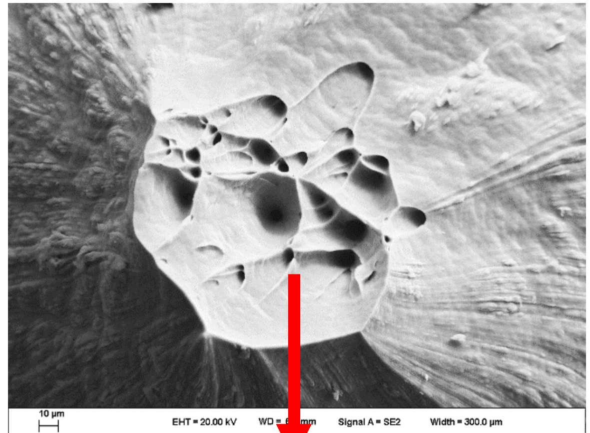
99.9% Al

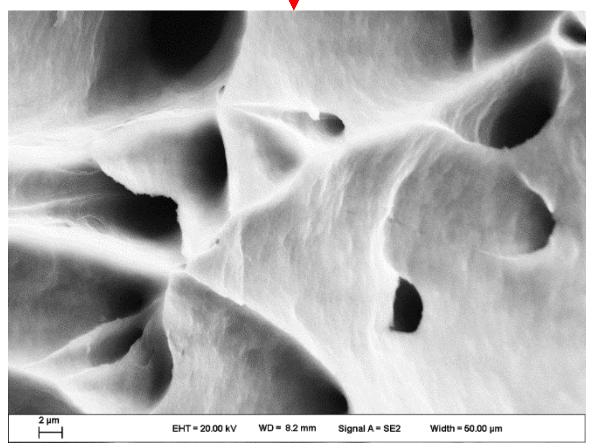




- Classic ductile dimples
- At least some void appear to nucleate at hard inclusions
- A potential case study for hard particle nucleation?

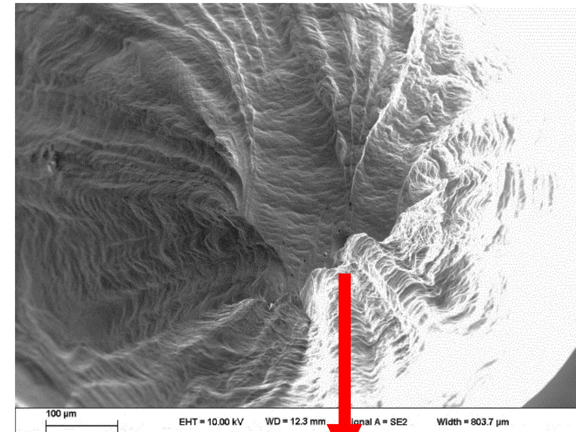
99.99% Al

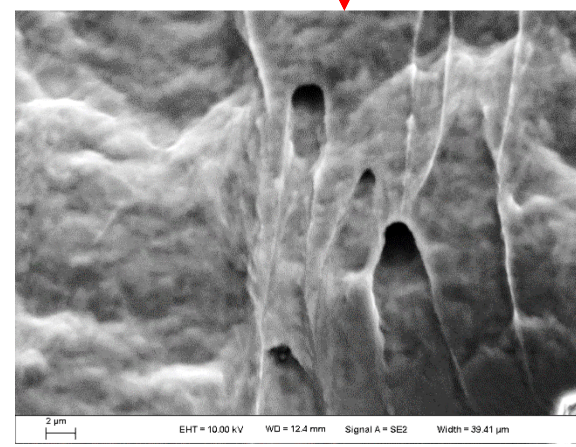




- **“goldilocks zone”** for pure initiation?
- Avoids dynamic recrystallization & nucleation at inclusions

99.999% Al

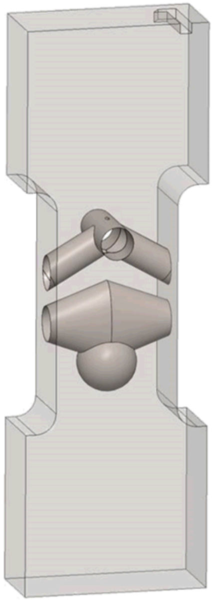




- Necking to a point (100% reduction in area)
- Only a few dimples at rupture
- Cross-sections reveal dynamic recrystallization

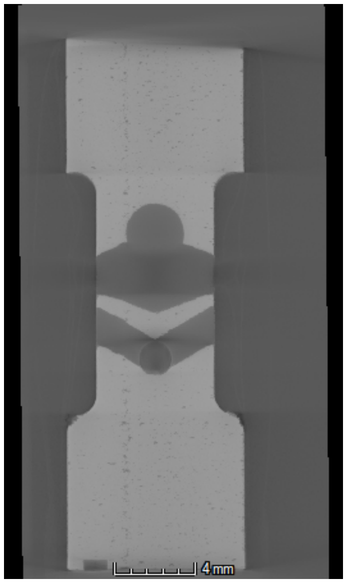
Underway… The 3rd Sandia Fracture Challenge

An additively manufactured structure with internal chambers that cannot be manufactured by conventional methods

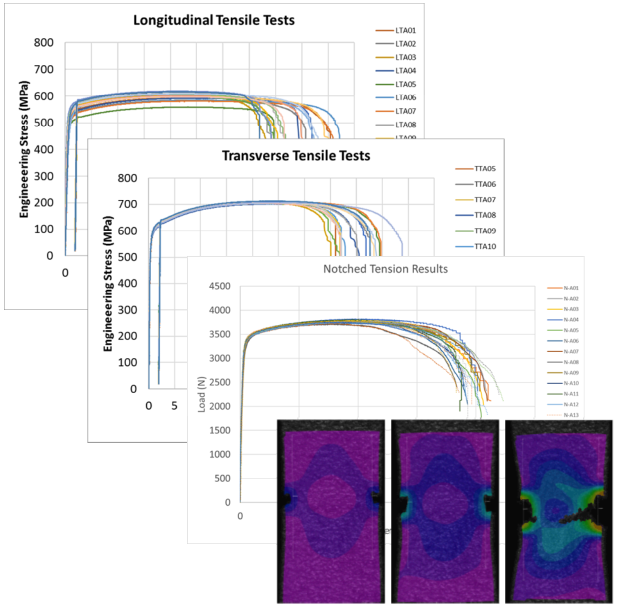


CAD

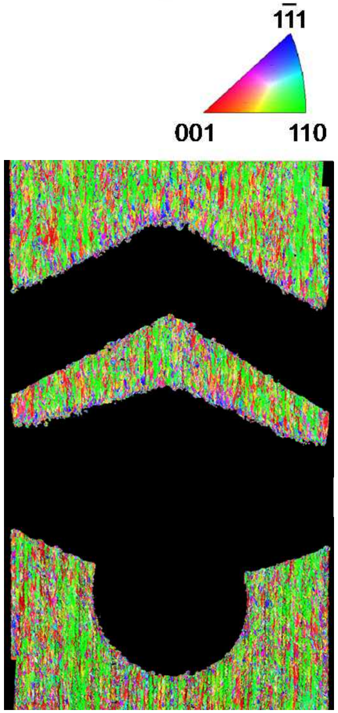
Optical Image



CT Scan showing internal porosity



Notch & smooth bar calibration data (with DIC) from the same build



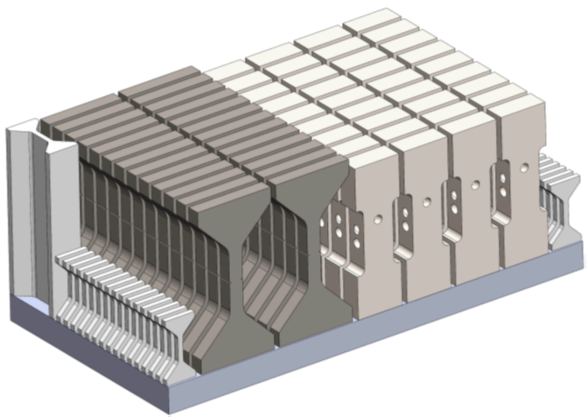
Microstructure & Texture data

Provided the following engineering data…

- x-ray CT scans
- tensile & notch tensile tests
- EBSD Microstructure, surface roughness, etc.

Predict the variability in failure response…

- location of crack initiation
- forces associated with crack initiation
- local surface strains during deformation



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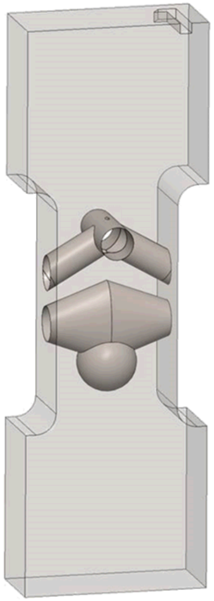
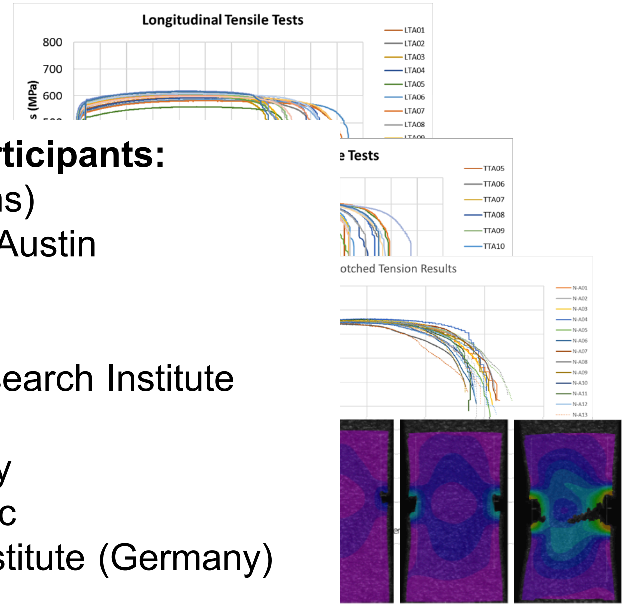
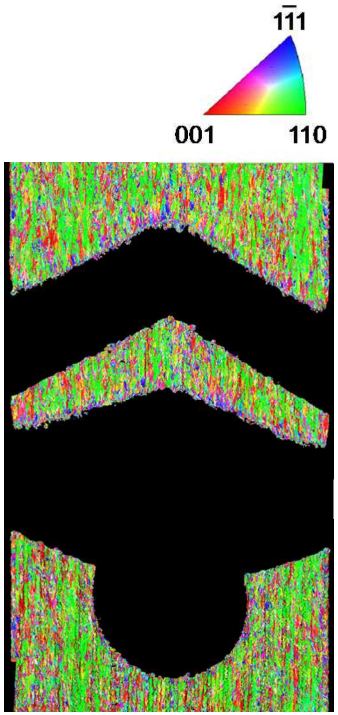


CAD

Optical Image



ar calibration
n the same build



Microstructure & Texture data

Pre-registered Participants:

1. Sandia (3 teams)
2. Univ. of Texas-Austin
3. MIT
4. Purdue
5. Southwest Research Institute
6. Exponent
7. Pratt & Whitney
8. General Electric
9. Max-Planck Institute (Germany)
10. Univ. of Utah
11. OCAS NE (France)
12. RWTH Aachen (Germany)
13. Thinkviewer
14. Regensburg Univ. (Germany)
15. Kazimierz Wielki Univ. (Poland)
16. Tecnalia Research (Spain)
17. US Army Corps of Engineers
18. US Army ARDEC

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EBSD Microstructure,

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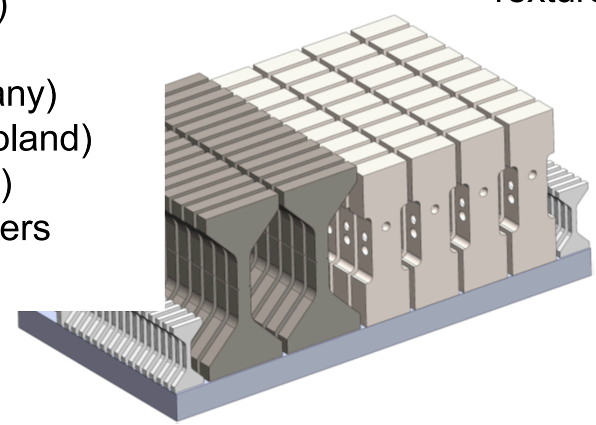


Sandia National Laboratories

The purpose of the Structural Reliability Partnership is to leverage expertise and investments from multiple institutions on areas of mutual interest in the domain of structural reliability.

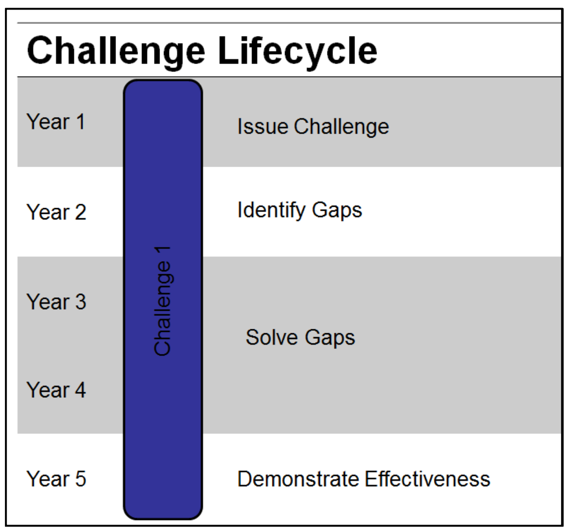
Preliminary pilot partners:

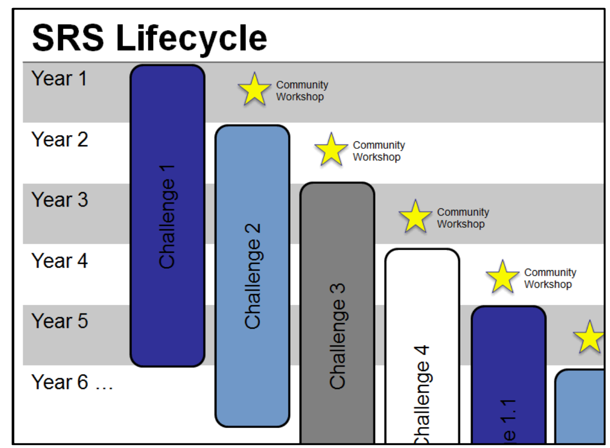
Sandia National Laboratories

ExxonMobil

Massachusetts Institute of Technology

TEXAS
The University of Texas at Austin





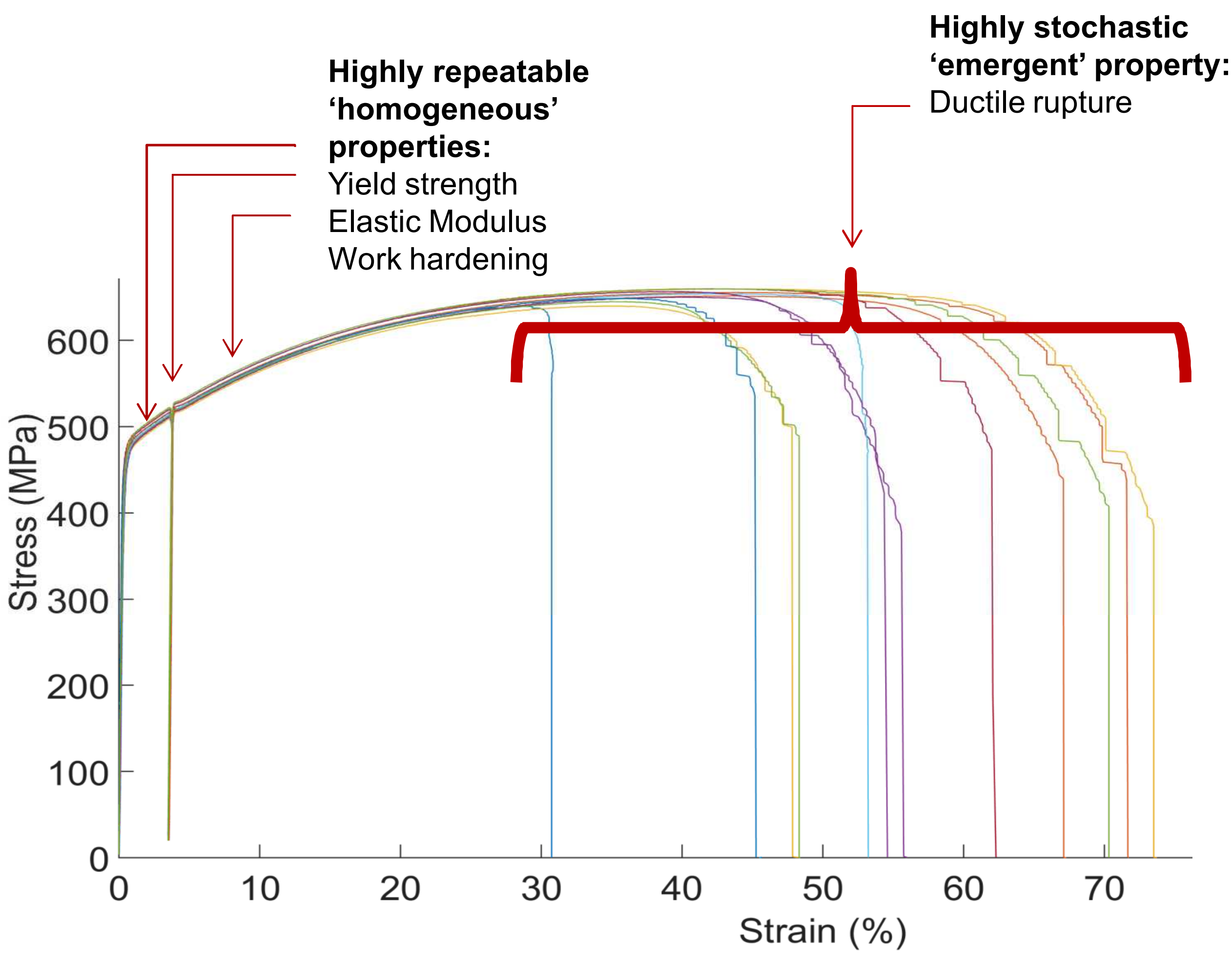
Sandia National Laboratories

Two general categories for material phenomena

Homogeneous vs. Heterogeneous (Emergent / Weakest Lin

(governed by average microstructure)	**(highly stochastic phenomena governed by a 'weak' feature in the microstructure)**
Elasticity	Ductile Rupture
Yield strength (engineering)	Corrosion Pit Initiation
Thermal Conductivity	Dielectric Breakdown
Electrical Conductivity	Creep Rupture
Magnetic Permeability	Nuclei in Solidification

Heterogeneous "Emergent" Phenomena are Particularly Challenging for Material R



12 Nominally Identical Additively Manufactured 304L Tensile Bars Produced by NSC