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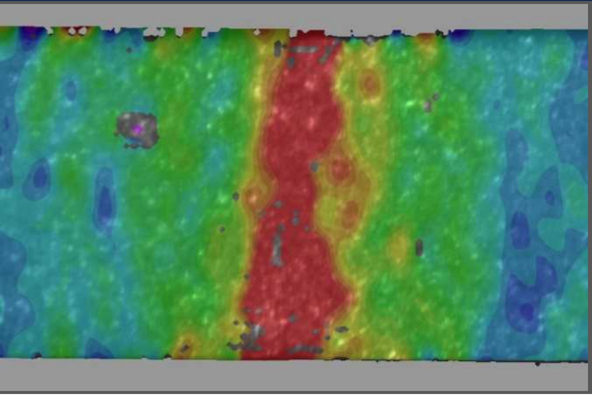

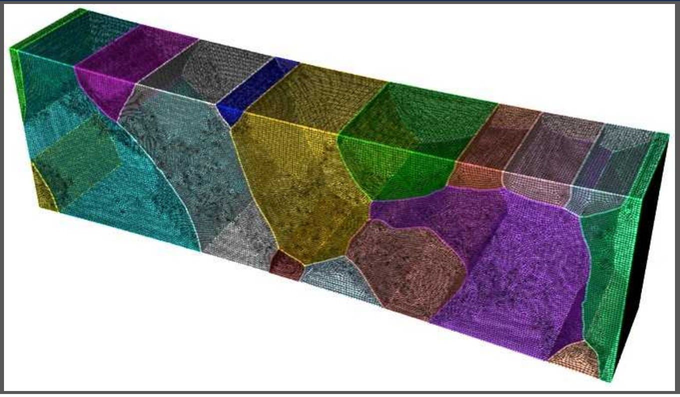

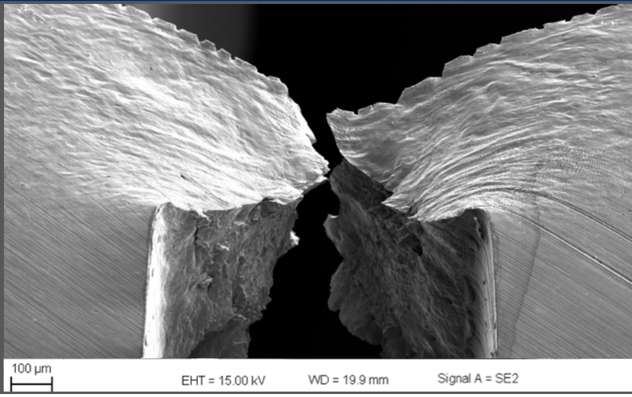

Characterization of Void-Dominated Ductile Failure in Pure Ta

B. G. Clark, J. R. Michael, B. B. McKenzie, J. Carroll, H. Lim, and B. L. Boyce

May 30th, 2016 • THERMEC 2016 • Graz, Austria

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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The Land of Enchantment


Sandia Mountains at Sunset

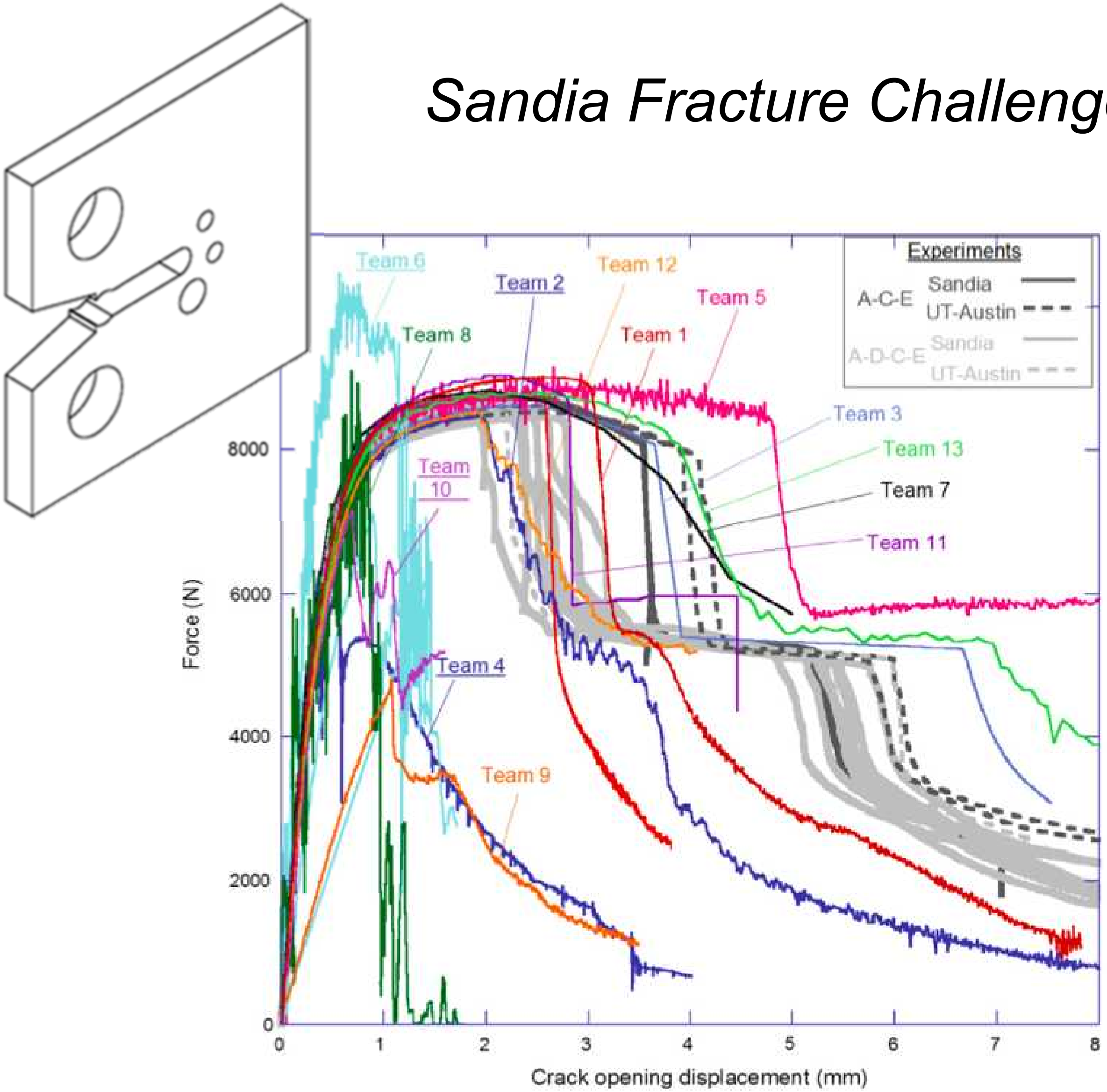
Balloon Fiesta


Green Chile

Sandia National Labs

Predictive Modeling is Challenging

Sandia Fracture Challenge →

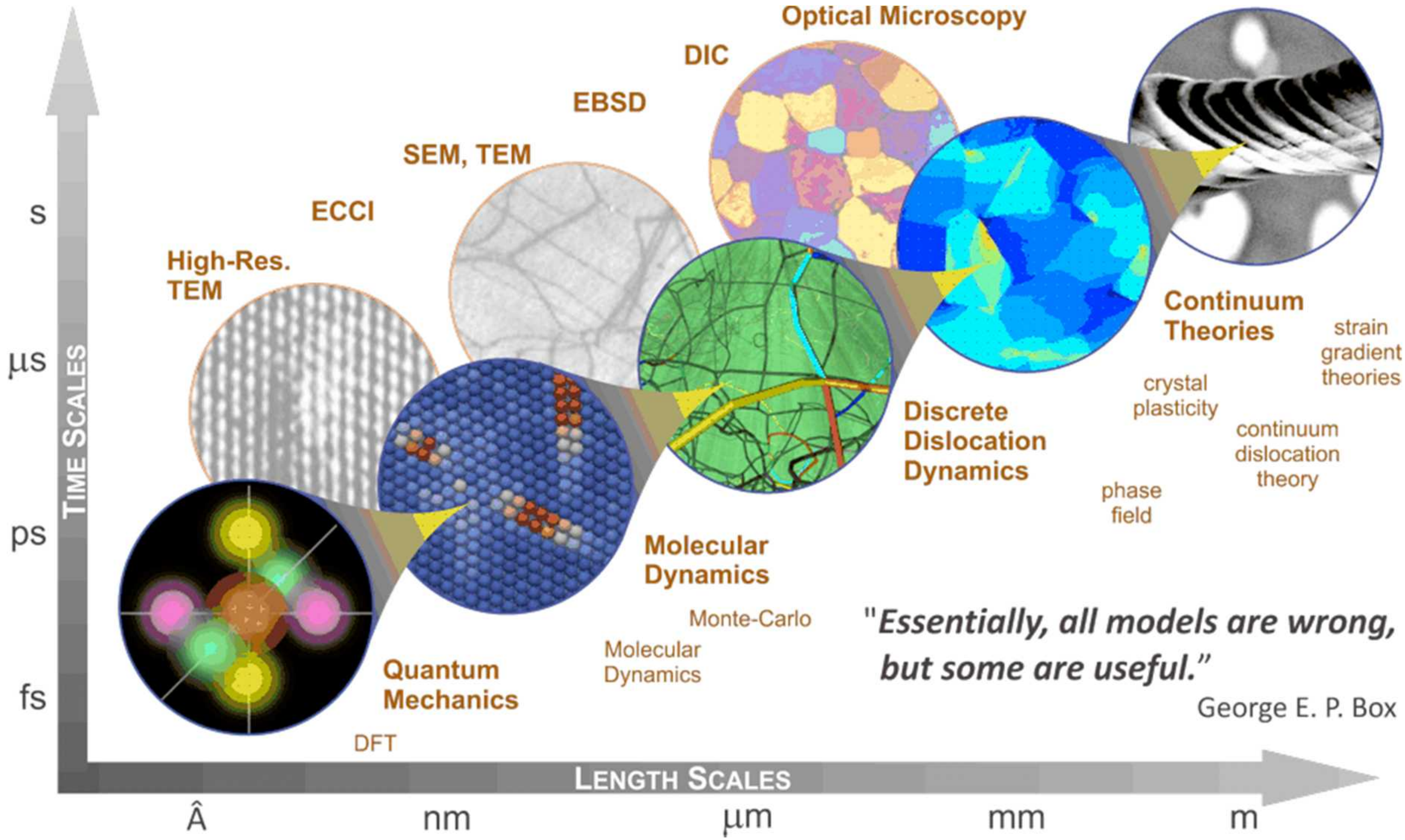


Teams asked to predict:

- Force and COD at which crack(s) initiate
- Path of crack
- 3 independent experimental labs collected data
- 13 groups gave predictions from models
- *Wide variety in predicted results*

B. L. Boyce et al., Int. J. Frac (2014).

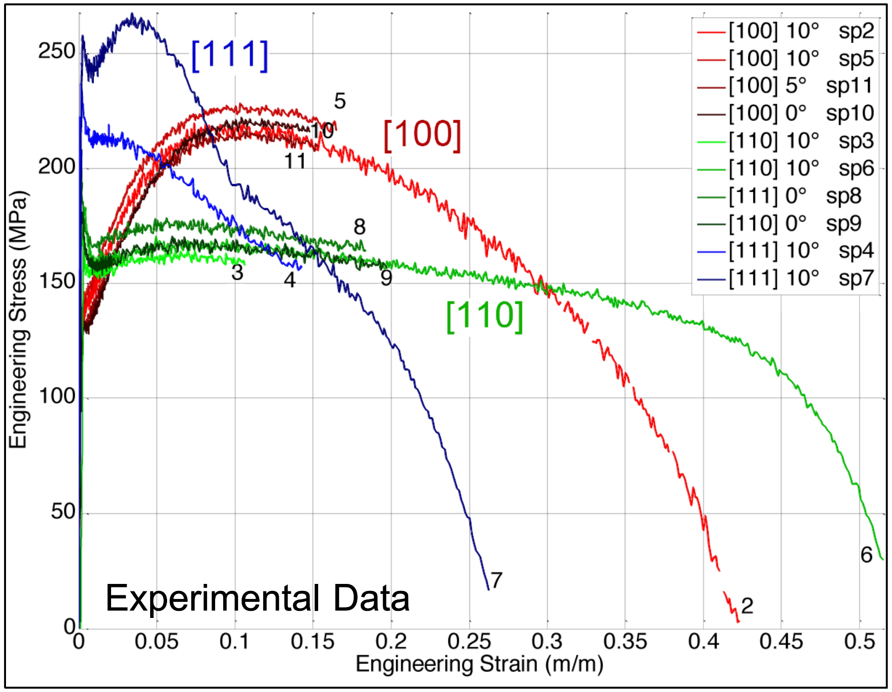
Microscopy Plays Key Role

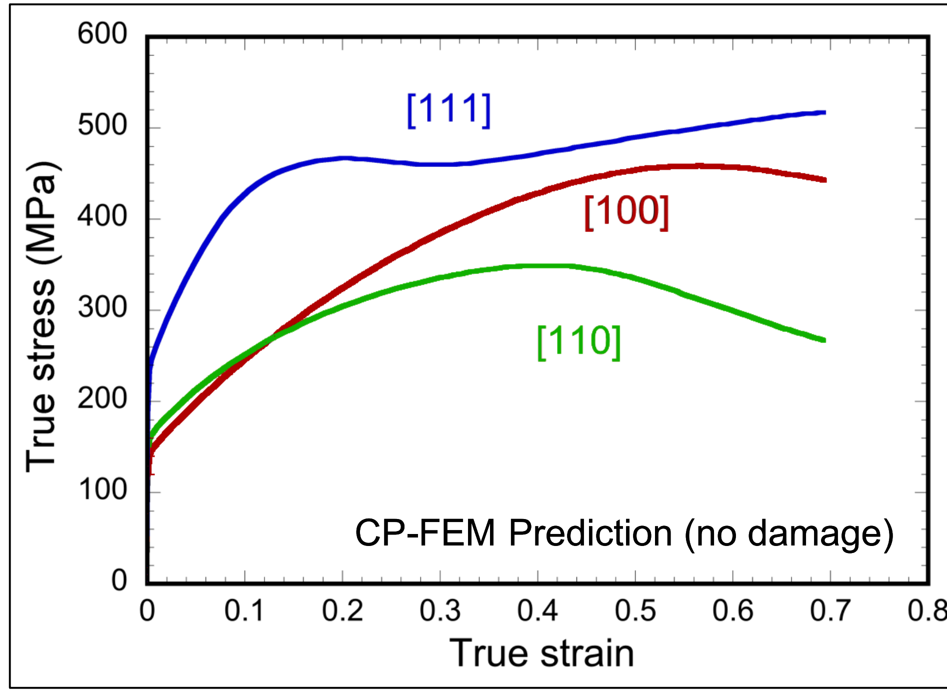


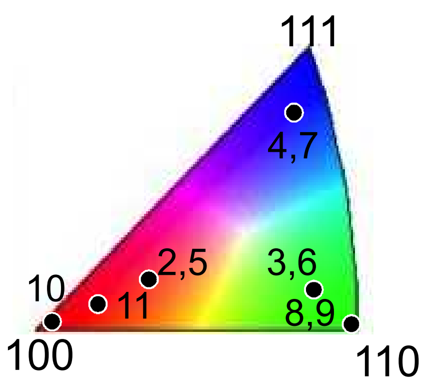
Experimental data provides physical basis for predictive simulation development

http://www.kochmann.caltech.edu/research_QC.html

Predicting Ductile Failure in Ta



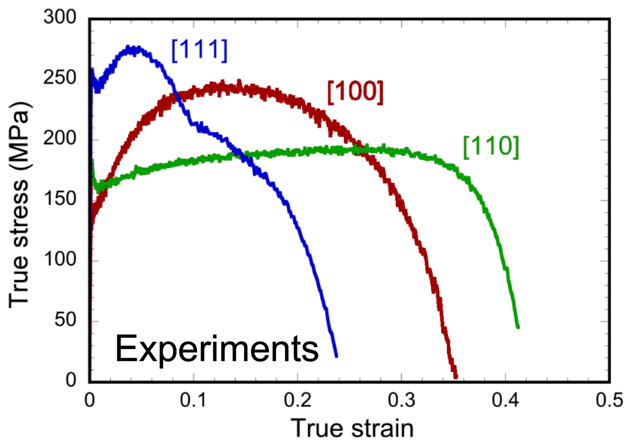




Without including damage in CP-FEM:

- No softening occurs other than necking
- The material does not “degrade” (e.g. voids, crack, tearing)
- Stress-strain response does not match experiments

Getting the Damage "Right"



*Metrics for Microstructurally Small Fatigue Crack (MSFC)**

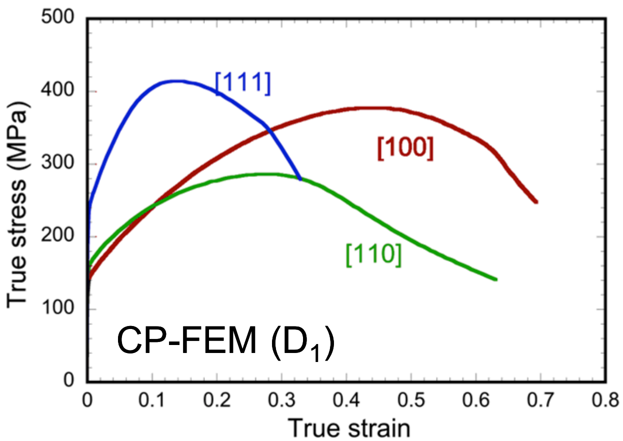
$$D_1 = \max_{\alpha} \int_0^t \left|\dot{\gamma}^{\alpha}\right| dt$$ (Max. accumulated slip over each slip system)

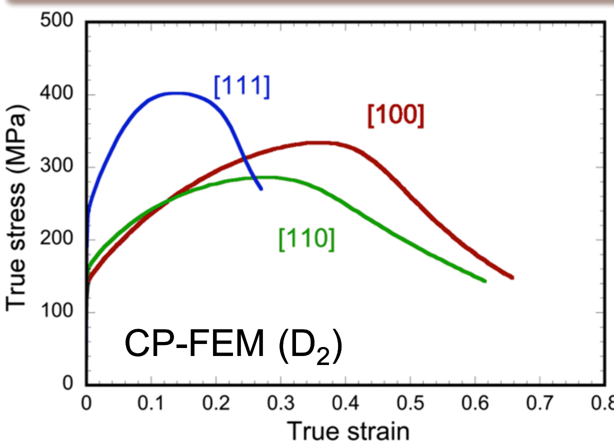
$$D_2 = \max_{p} \int_0^t \left|\dot{\gamma}^{p}\right| dt$$ (Max. accumulated slip over each slip plane)

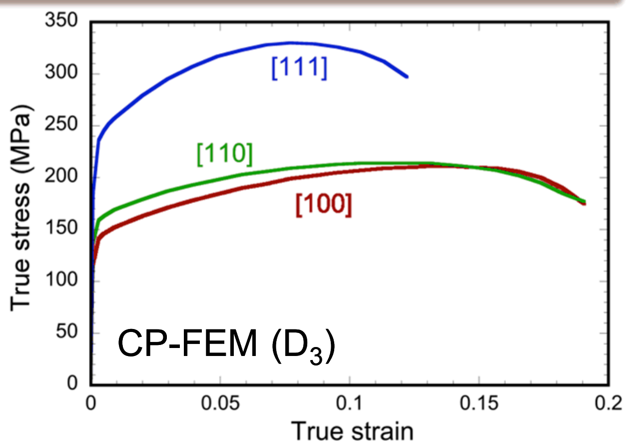
$$D_3 = \sum_{\alpha=0}^{N} \int_0^t \left|\dot{\gamma}^{\alpha}\right| dt$$ (Total accumulated slip over each slip system)

"Accumulated slip"

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha}}{(1 - D_i) g^{\alpha}} \right)^{1/m}$$





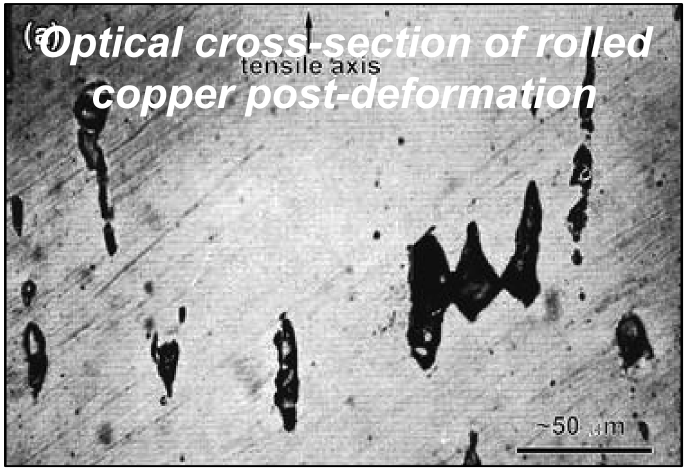


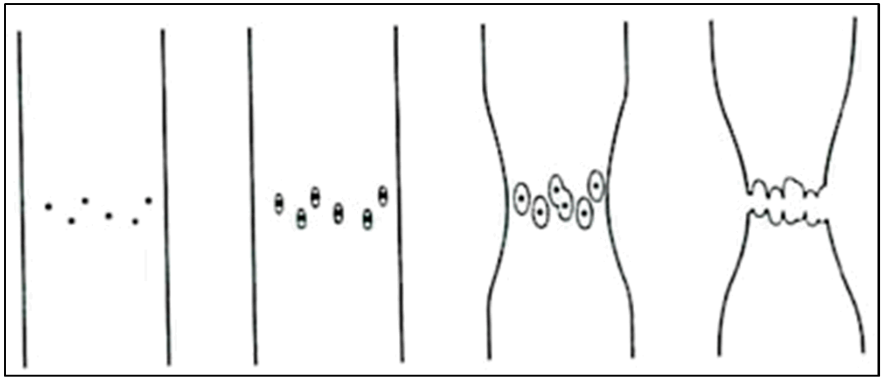
What controls the initiation of damage in Ta?
How can we better understand how damage nucleates and accumulates?

*J. D. Hochhalter et al., *Modelling Simul. Mater. Sci. Eng.*, 2010. v.18, 045004

Ductile Fracture Mechanism

- Mechanical description of void nucleation, growth, and coalescence largely based on studies in 50's and 60's
- Initiation of voids through decohesion at second-phase particles or inclusions
- Voids continue to grow in response to high stresses, eventually coalesce
- *In this study, 99.9% Ta used; no evidence of second-phases or inclusions via SEM/TEM*

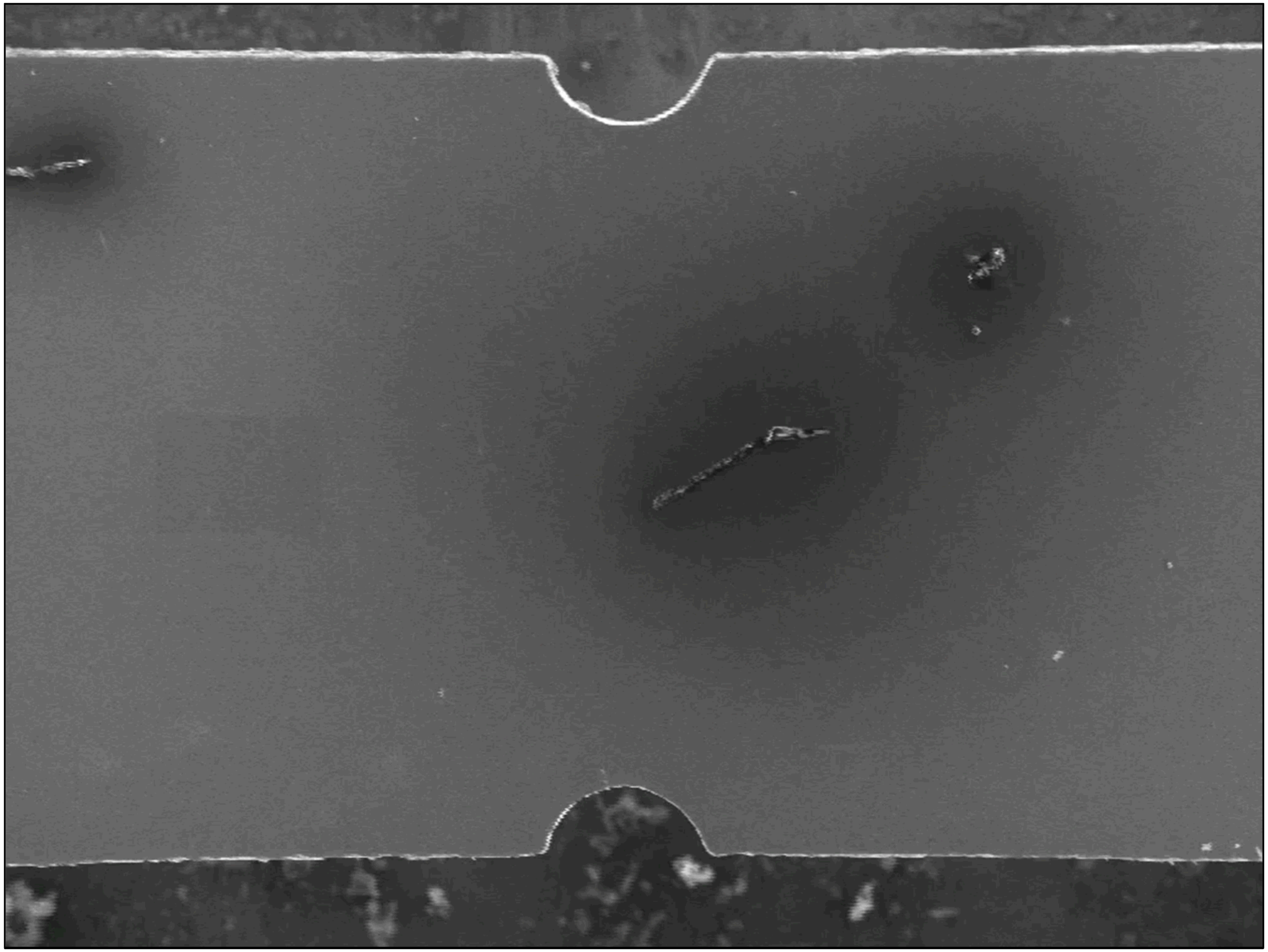




Can modern techniques reveal how voids initiate in pure metals?

Puttick, 1959; http://en.wikipedia.org/wiki/Fracture;

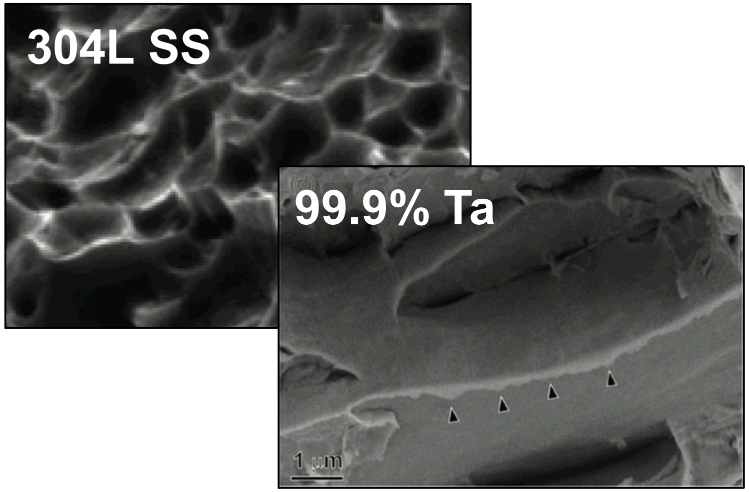
Tensile Testing of 99.9%Ta

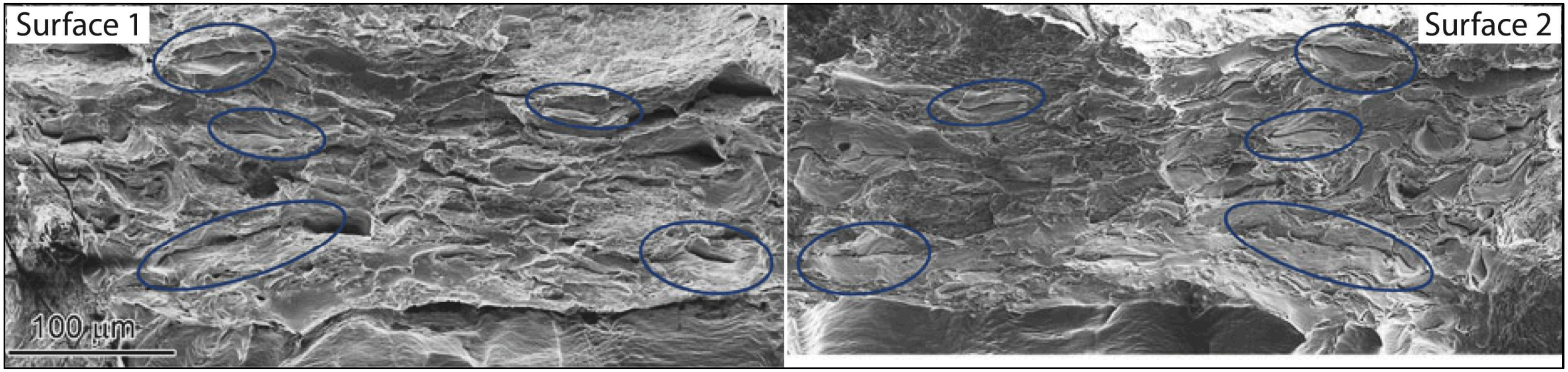


In Situ Scanning Electron Microscope (SEM) tensile test on Ta

Fractography of 99.9%Ta

- Ta exhibits significant ductility, but with valley/ridge fracture surface
  → no 'classic' hemispherical dimpling
- Mating surfaces are mirrored
  → with no evidence of cup-cone

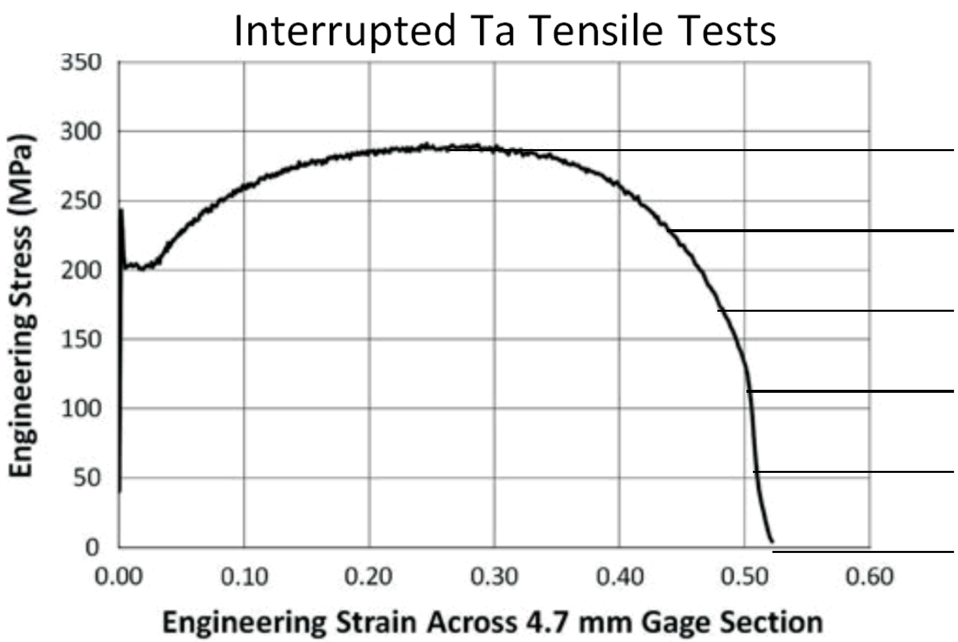


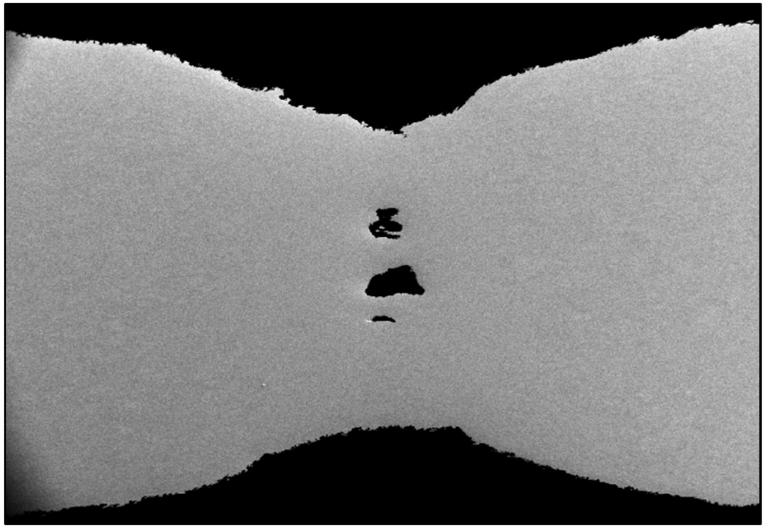


What role does local microstructure play in void initiation and growth?

Boyce, Clark, et al., Met Trans, 2013.

Characterization of Deformed Ta

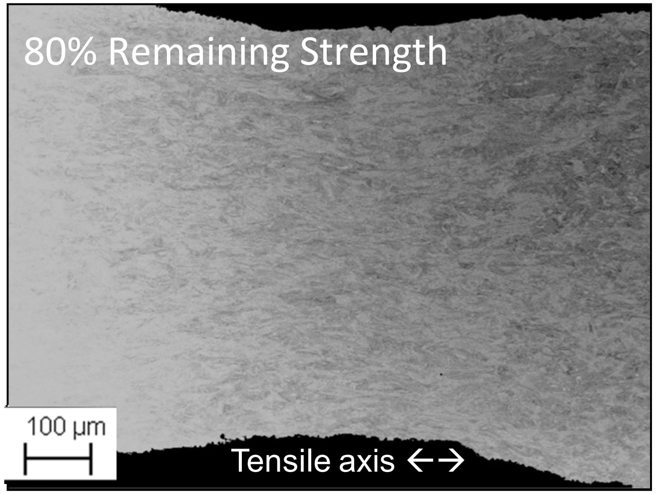




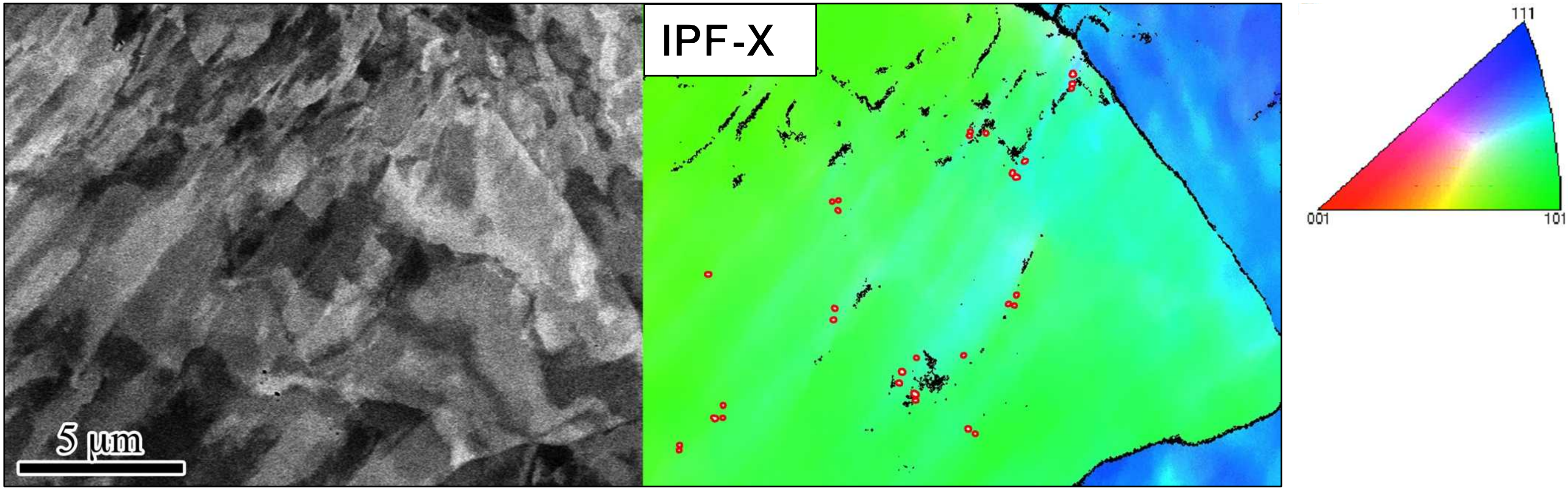
Ta tensile bar deformed at $5x10^{-3}$ to 40% remaining strength and polished to mid-plane for void analysis

Deformed Ta samples polished to mid-plane to investigate local microstructure in voided regions

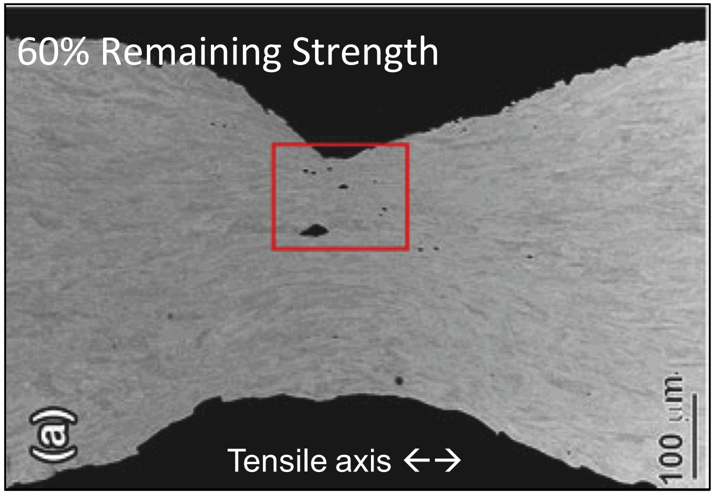
Void Formation at 80% RTS



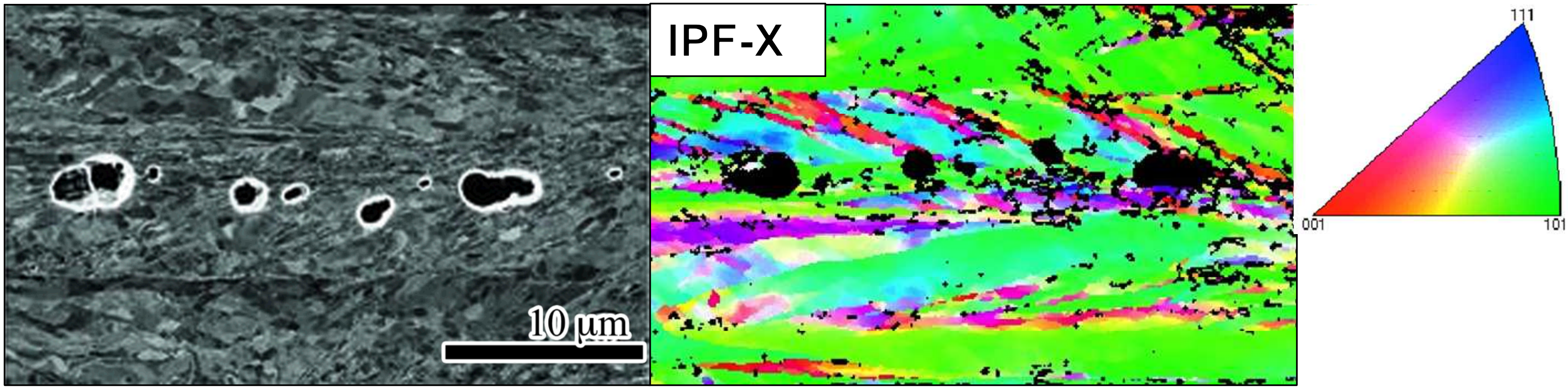
- Sample has begun to neck
- No large voids observed
- EBSD shows scattered small voids (30-100 nm) near bands of [122] / [110] aligned with tensile axis



Void Formation at 60% RTS



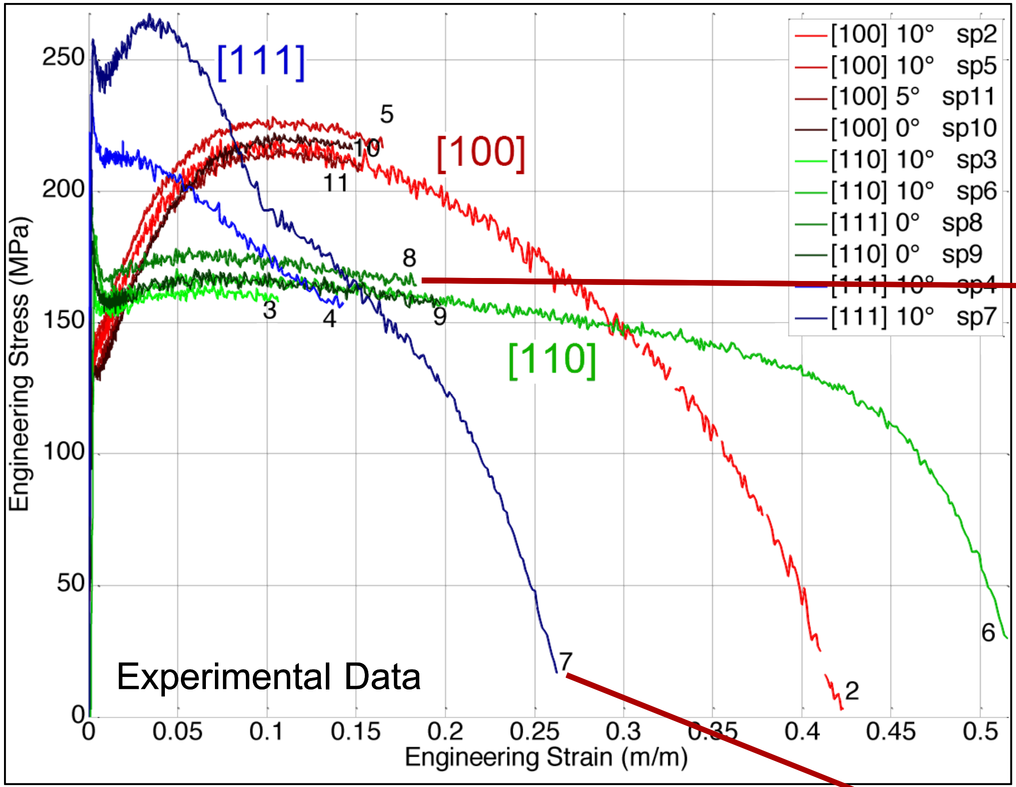
- Arrays of voids aligned along tensile axis
- EBSD shows elongated, inclined [001] subgrains associated with each void
- Alternating regions of [122] indicates high angle GBs

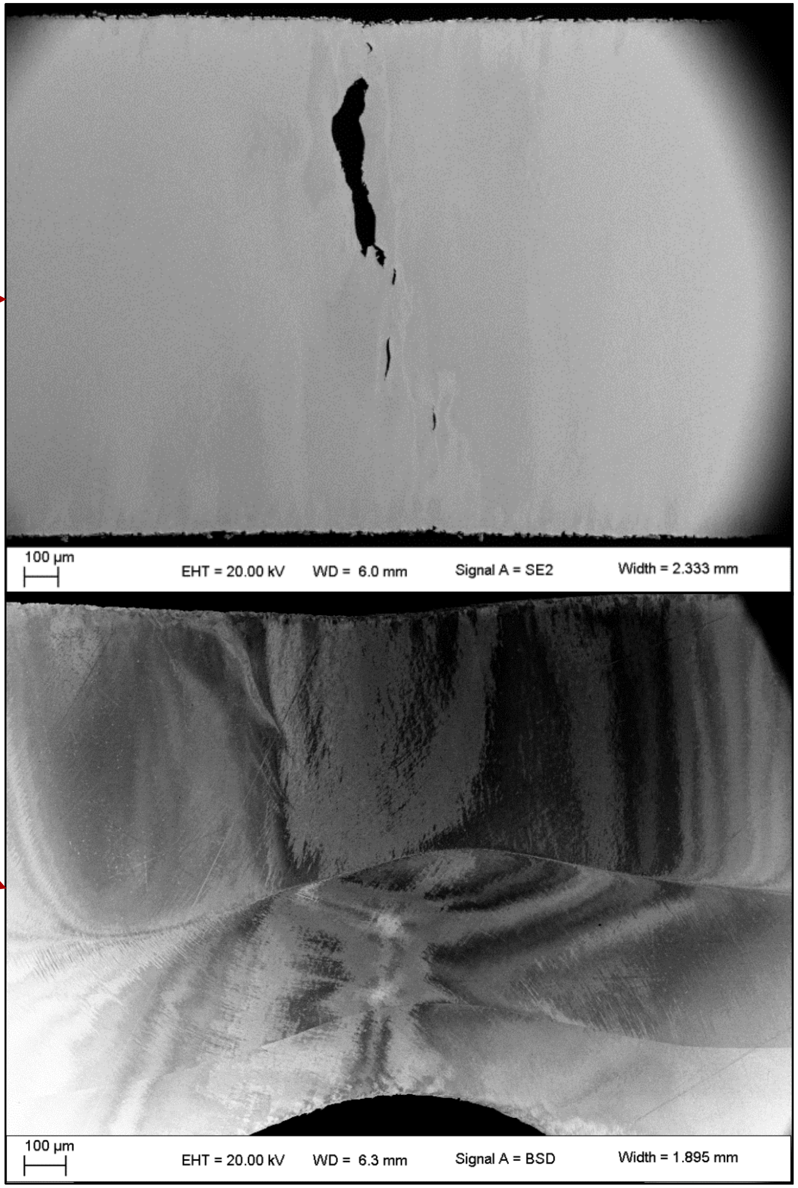


Deformation-induced microstructural changes and stress state controls the initiation/growth of voids

Boyce, Clark, et al., Met Trans, 2013; B. G. Clark et al., unpublished.

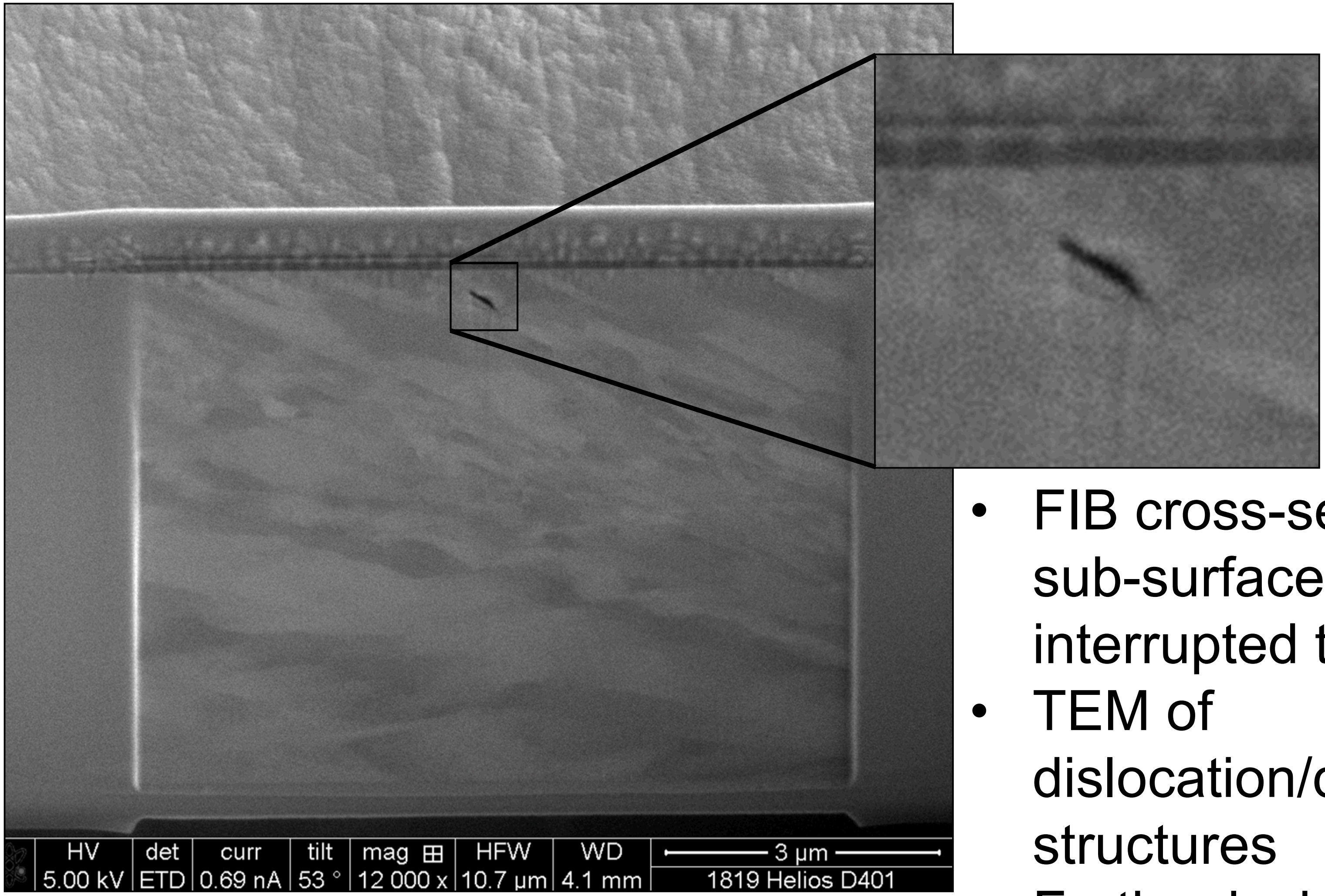
Void Formation in Single Crystal Ta





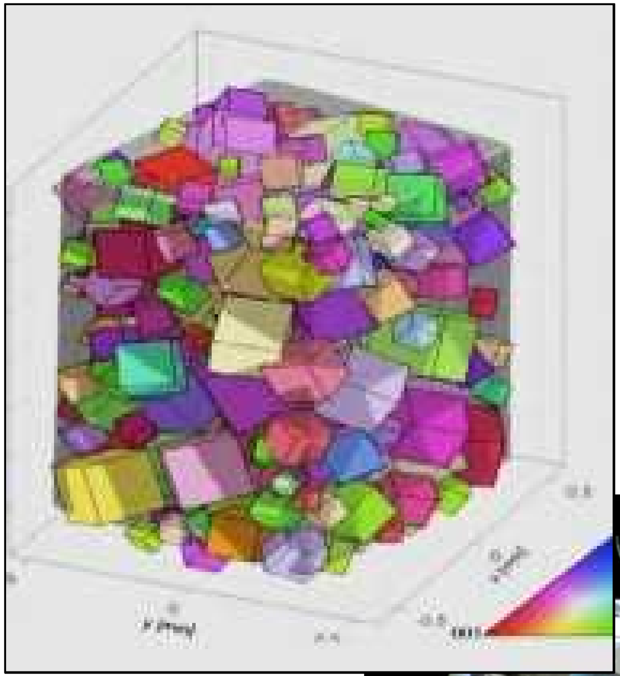
- [110] Ta shows void formation well before failure
- [111] Ta shows necking, but no evidence of voiding, right up to point of failure

Future Work: TEM of Voids in Ta

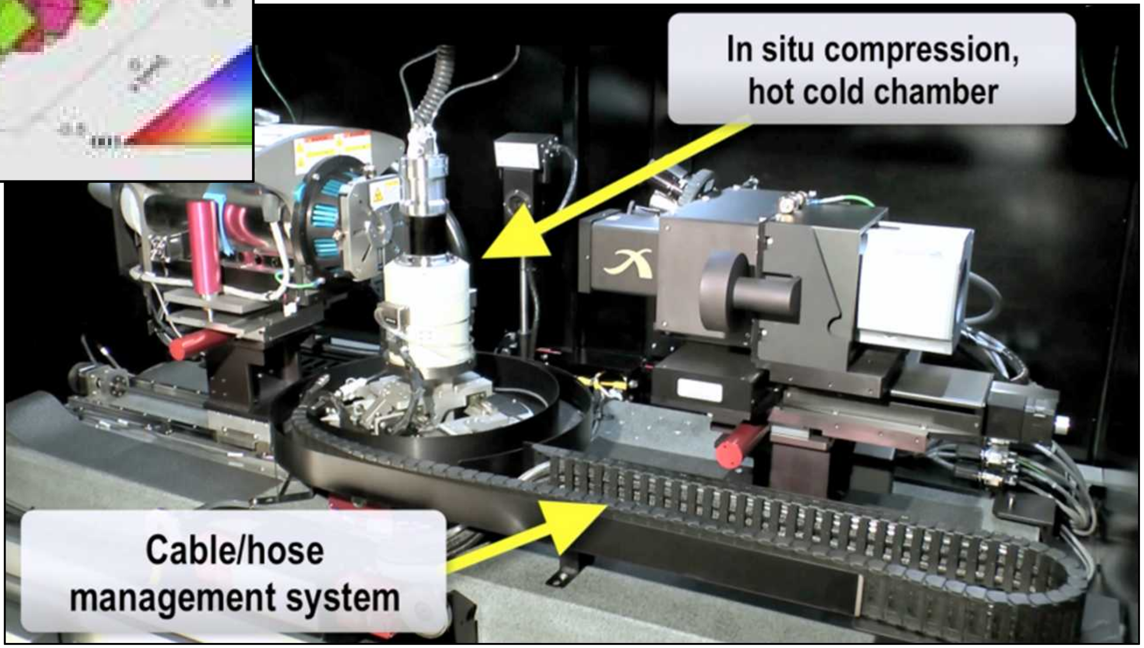


- FIB cross-sections of sub-surface voids in interrupted tensile bars
- TEM of dislocation/defect structures
- Further insight into void nucleation mechanism

Future Work: X-Ray Tomography



- Diffraction contrast tomography to map grain orientations in Ta tensile bar
- Deform in-situ with 3D x-ray tomography to map void evolution
- Compare 1:1 experimental and modeling results from **same** starting microstructure



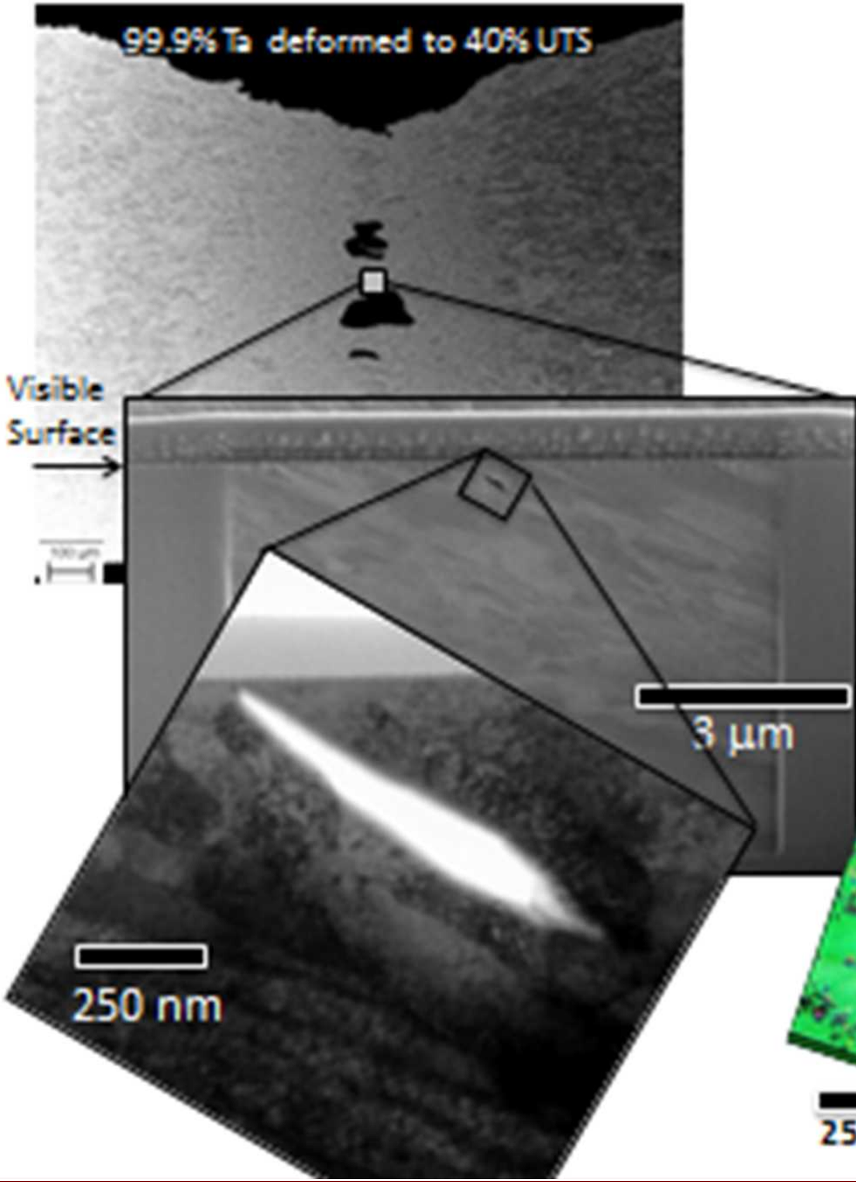
Conclusions

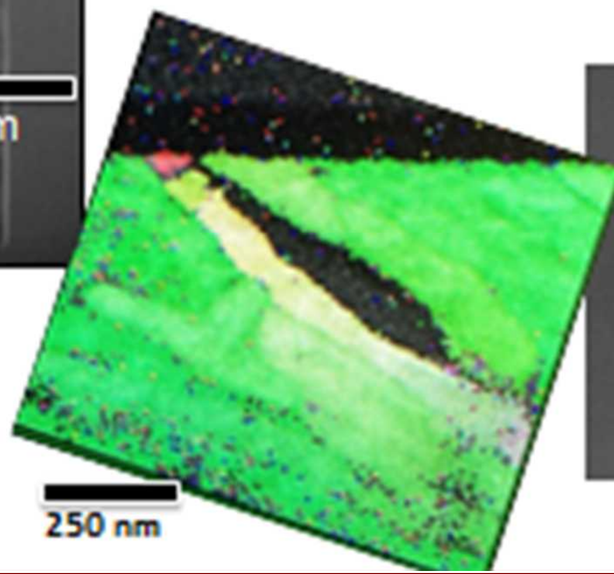
- 99.9% pure Ta is ductile, but does not exhibit a ‘classic’ ductile fracture surface (i.e. hemispherical dimples)
  → but, fracture surface still indicates void-driven failure
- Voids in interrupted tensile test specimens were analyzed by SEM and EBSD
  → voids prevalent in regions of high misorientation
- No inclusions or second-phases observed via SEM or TEM
  → void initiation likely at dislocation junctions / sub-boundaries
- Early single crystal Ta results are consistent with polycrstalline results: Grains oriented as [110] form voids readily in Ta

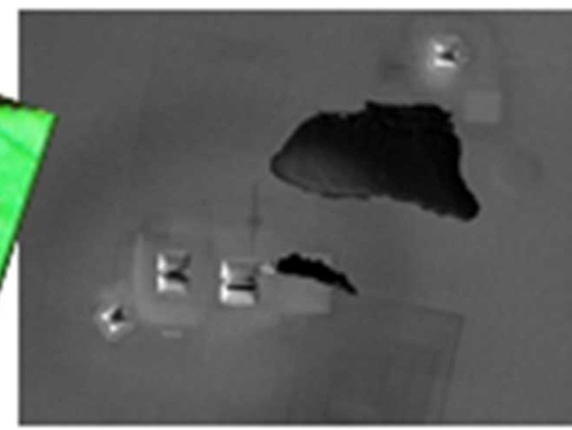
Failure mechanism of Ta is void-driven, with deformation-induced microstructural changes and stress state controlling the initiation and growth of voids

Nanoscale Analysis of Void Initiation

- Focused Ion Beam (FIB) used to locate subsurface, deformation-induced voids in interrupted tensile bar.
- Preliminary TEM shows void shape aligned with angle of sub-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







Damage model in crystal plasticity

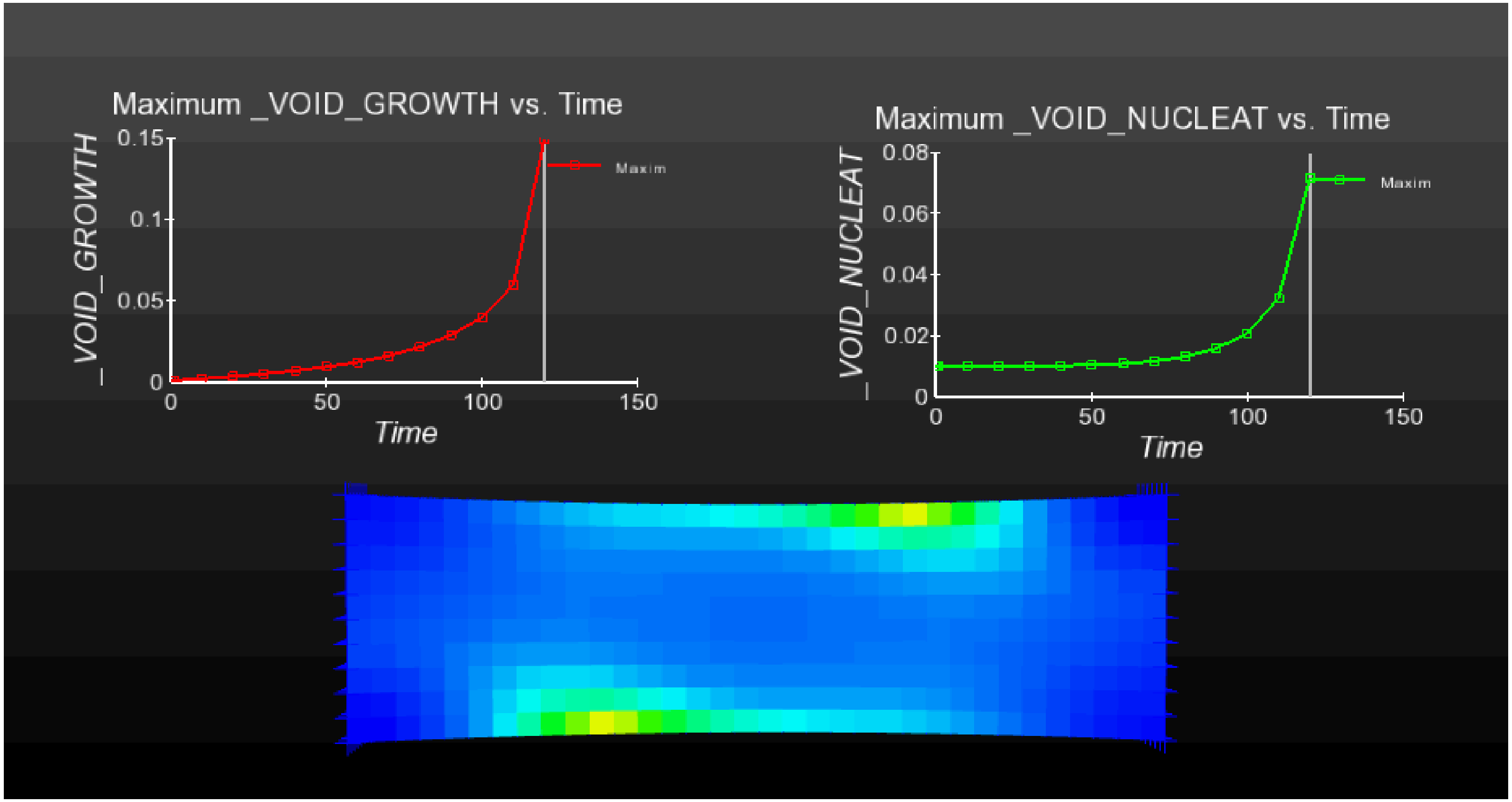
- Damage

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

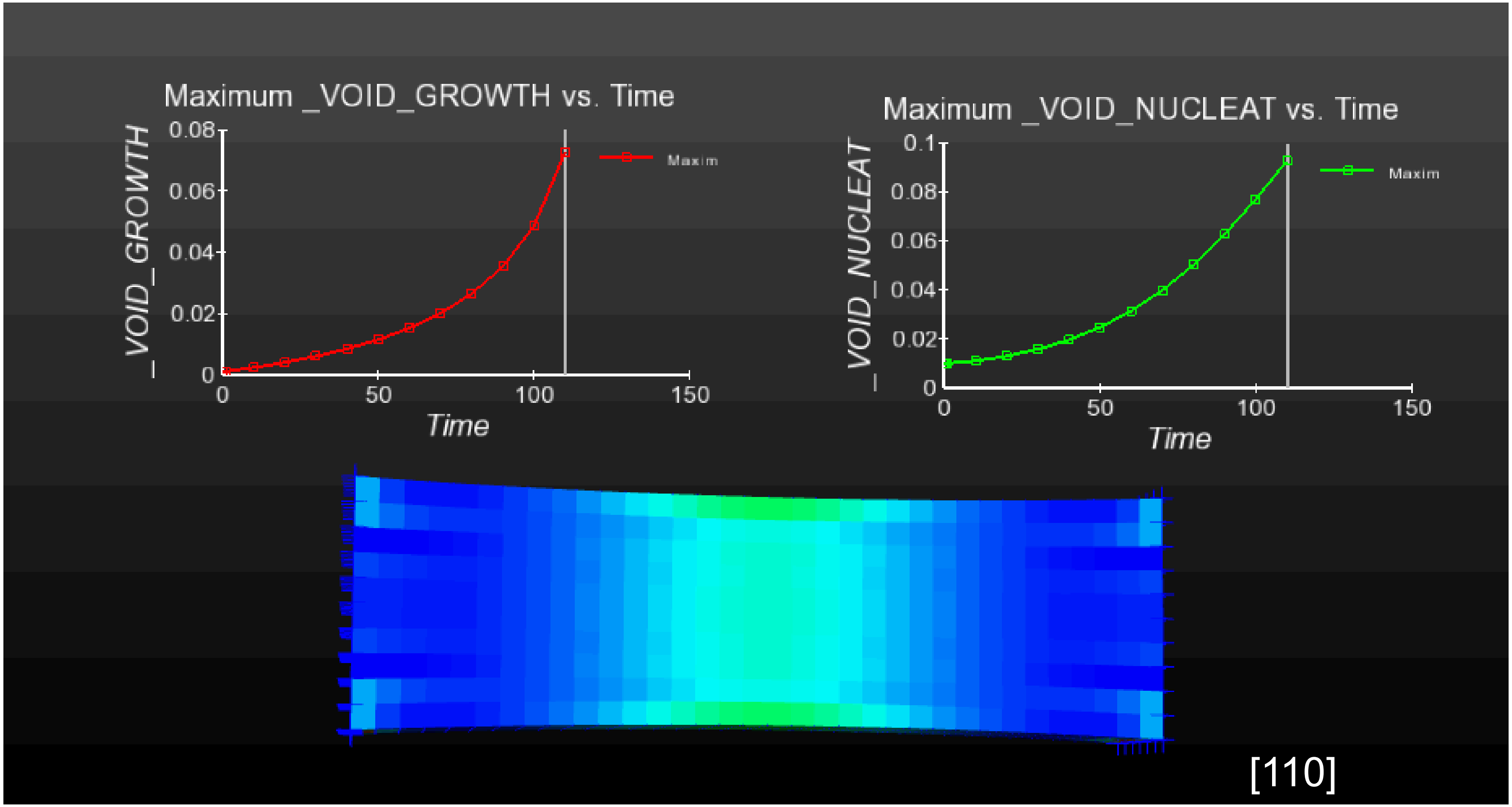
- Constitutive model

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{\tau^\alpha}{(1-\phi)g^\alpha} \right)^{1/m}$$

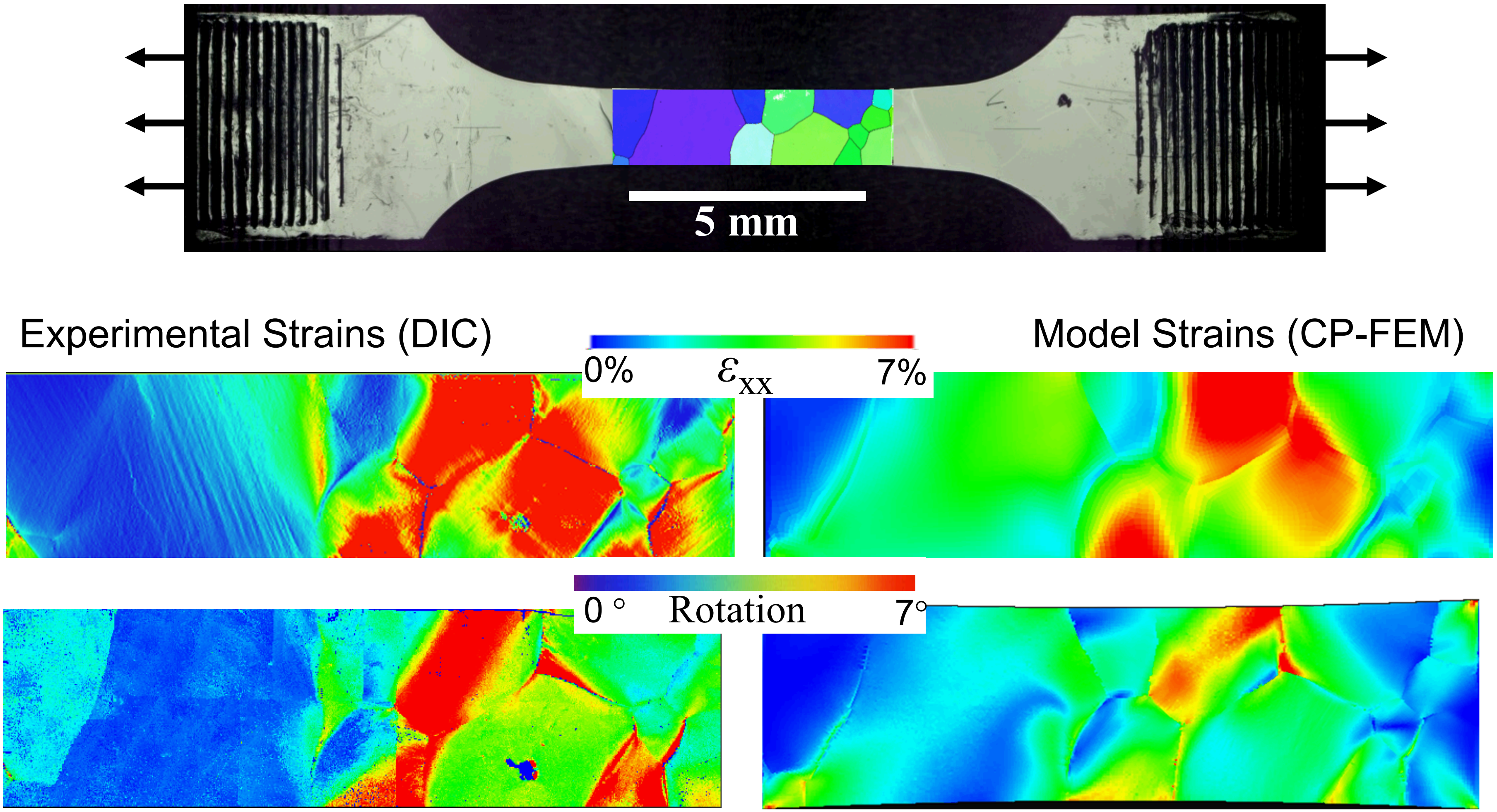
Ta single crystal simulation: [111]



Ta single crystal simulation: [110]



Crystal Plasticity Predictions



Great comparison *qualitatively*, but strain and rotation are underpredicted