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Temperature and Strain Rate Effects on the Dislocation Plasticity of BCC Transition Metals

H. Lim[1], J. D. Carroll[2], C. R. Weinberger[3], B. L. Boyce[2] and C. C. Battaile[1]

[1]Computational Materials & Data Science, [2]Metallurgy & Materials Joining
Sandia National Laboratories

[3]Department of Mechanical Engineering & Mechanics,
Drexel University

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Outline

- **Introduction**
- **Kink-Pair Theory**
- **CP-FEM Predictions**
- **Continuum-Scale Polycrystal Models**
- **Validation with Experiments**
- **Summary**

Introduction

Motivation for developing temp./ strain rate dependent BCC models

- ❖ BCC metals are of scientific and engineering interest
  - o Refractories/ High energy applications: W, Mo, Ta
  - o Structural materials: Steel

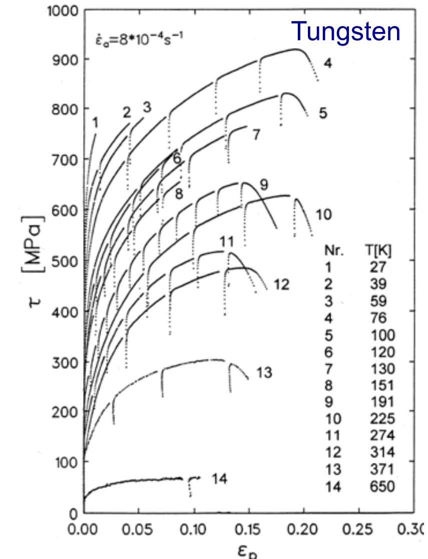
- ❖ Underrepresented in computational materials science studies
  - o Most models are phenomenological
  - o Complex response compared to FCC
    - \- Ambiguity of slip systems, non-Schmid effects
    - \- Temperature & strain rate dep. flow stress

$$\tau(T,\dot{\gamma}) = \underbrace{\tau^{*}(T,\dot{\gamma})}_{\text{Thermal}} + \underbrace{\tau_{obs}}_{\text{Athermal}}$$

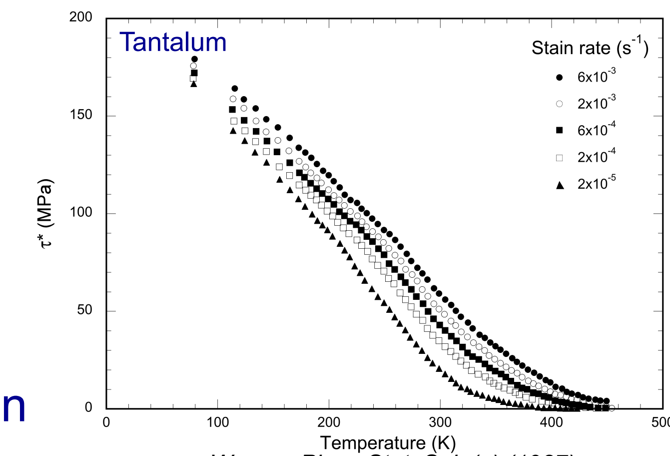
In FCC metals, $\tau^{*} \approx 0$

In BCC metals, $\tau^{*} >> 0 \qquad (T << T_c)$

Need a model of the resistance to slip by lattice friction



Brunner & Glebovsky Mat. Sci. Lett. (2000)



Werner, Phys. Stat. Sol. (a) (1987)

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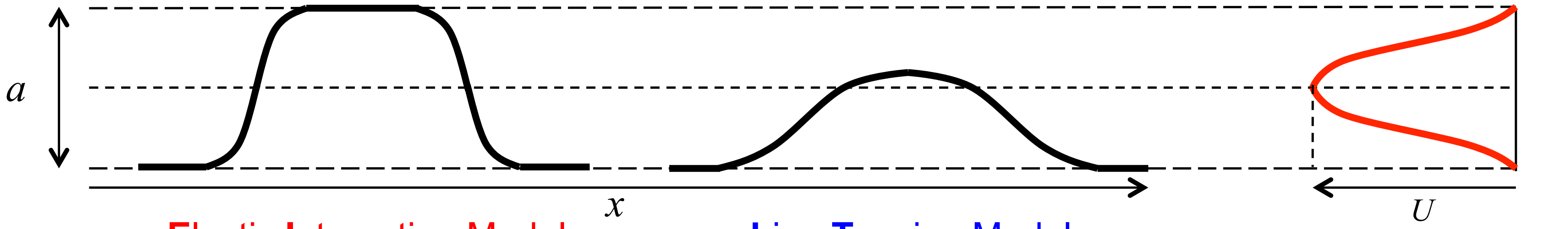
Kink-Pair Theory

Regime I (High T / low σ) | Regime II (Low T / High σ) | Peierls potential



Elastic Interaction Model

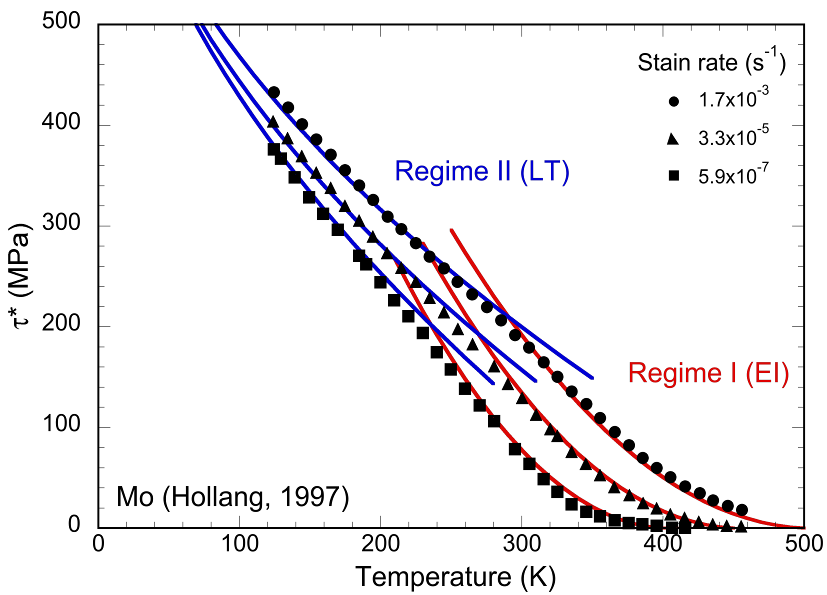
$$\tau^*_{EI}(T,\dot{\gamma}) = \tau_0^{EI}\left(1-\frac{T}{T_c(\dot{\gamma})}\right)^2$$

Line Tension Model

$$\tau^*_{LT}(T,\dot{\gamma}) = \tau_{LT}^{0}\left(1-\left(\frac{T}{T_c(\dot{\gamma})}\right)^{1/2}\right)$$

(Antiparabolic Peierls potential)

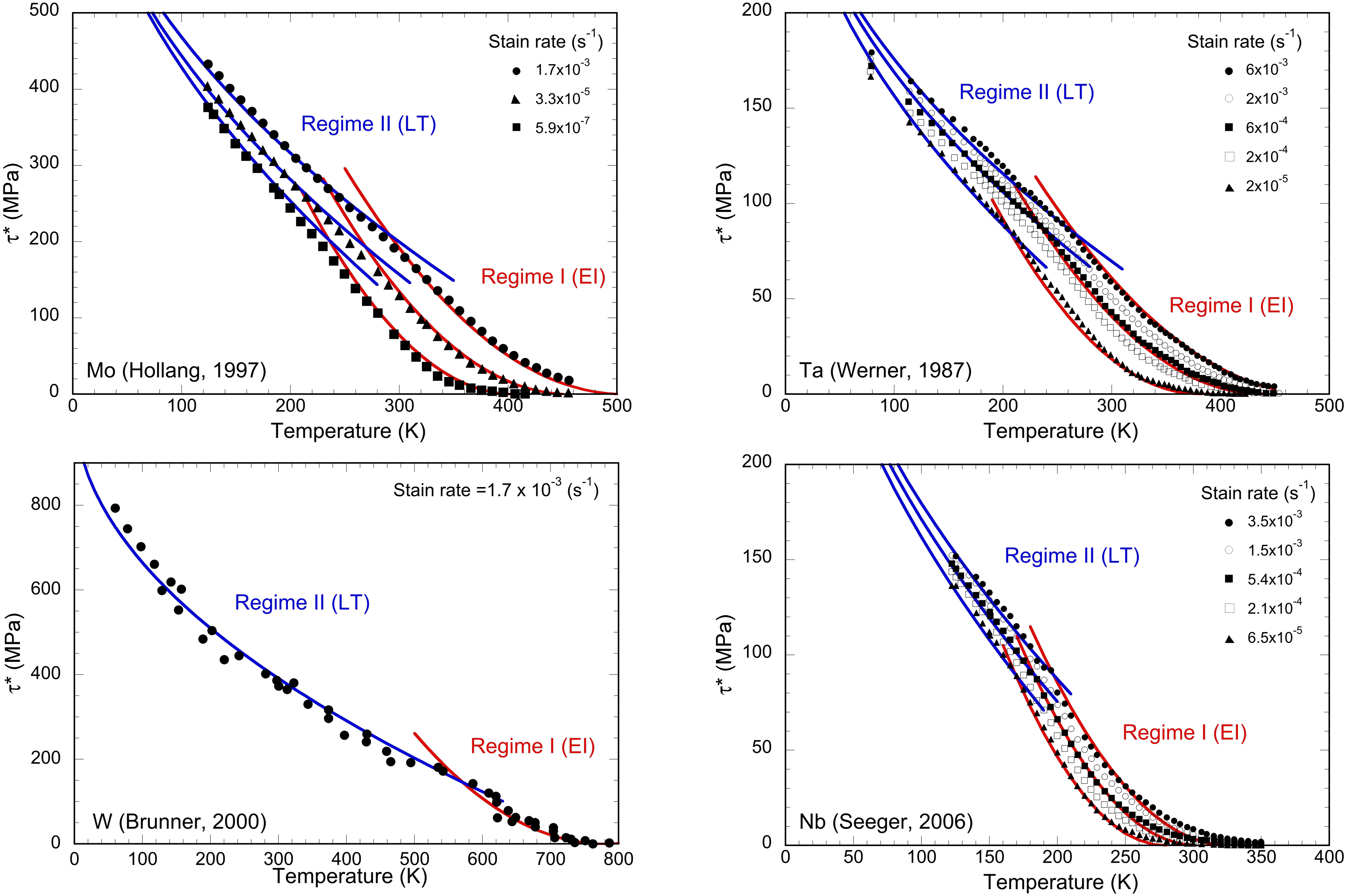
$$T_c(\dot{\gamma}) = \frac{2H_k}{k_B \ln\left(\dot{\gamma}_0/\dot{\gamma}\right)}$$



Best-fit material parameters

Material	$\dot{\gamma}_0$ (s^{-1})	$2H_k$ (eV)	τ_0^{EI} (MPa)	τ_0^{LT} (MPa)
Mo	3.75×10^{9}	1.27	1156	835
Ta	2.99×10^{6}	0.85	406	320
W	3.71×10^{10}	2.06	2035	1038
Nb	1.14×10^{8}	0.68	576	402

Measured and Fitted τ^*



Measured τ^* are accurately reproduced by the EI and LT models

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BCC CP-FEM Formulation

- FEM code developed at Sandia National Laboratories (JAS-3D)
- 24 {110}<111> slip systems
- Slip rate: $\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\dfrac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$ (Hutchinson, 1976)
- Slip resistance: $g^{\alpha} = \min\left(\tau_{EI}^{*\alpha}, \tau_{LT}^{*\alpha}\right) + \tau_{obs}^{\alpha}$

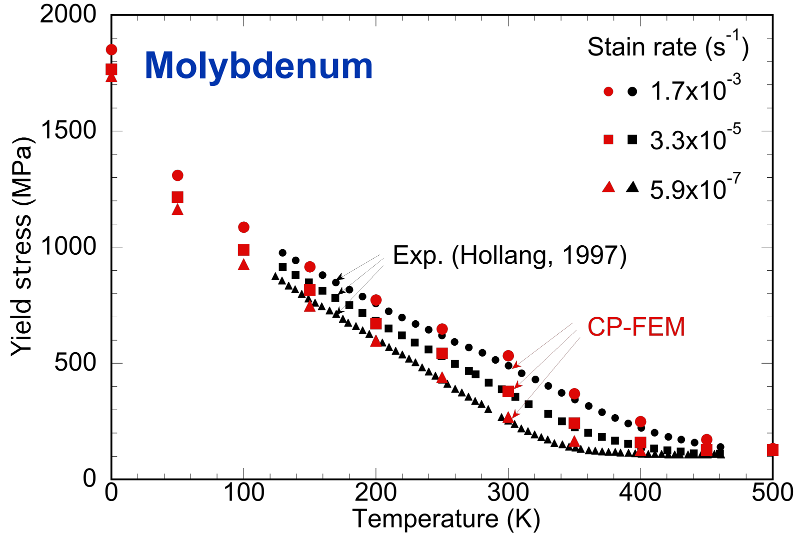
  Obstacle stress

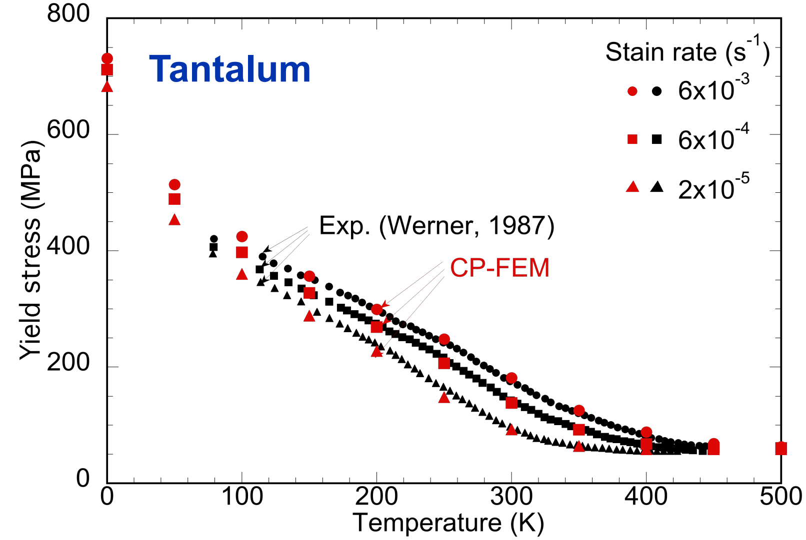
  Lattice friction

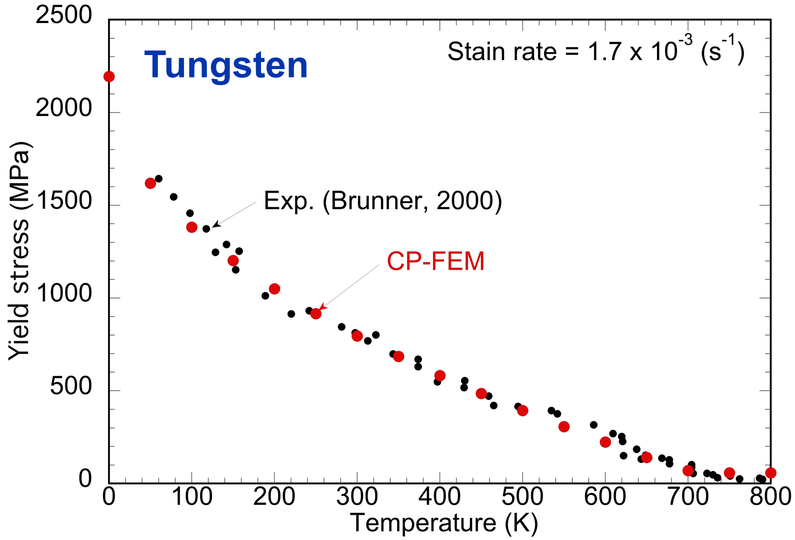
- Obstacle stress: $\tau_{obs}^{\alpha} = A\mu b \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}}$ (Taylor, 1934)

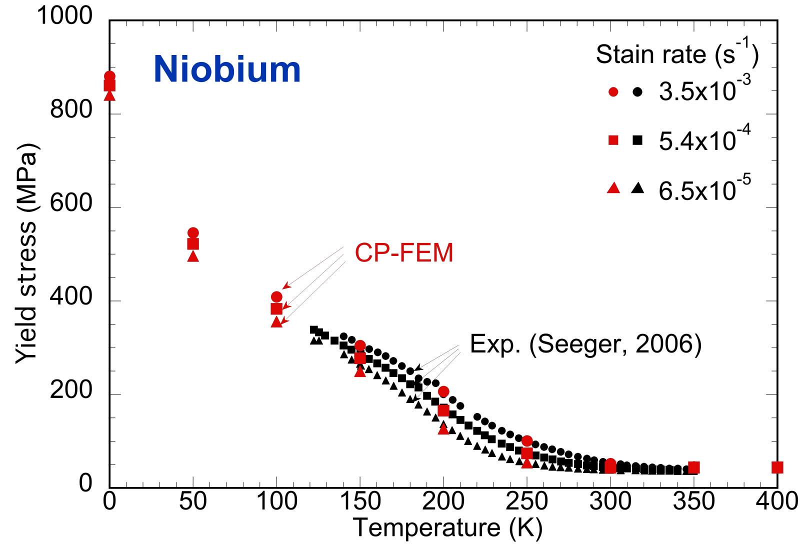
$$\dot{\rho}^{\alpha} = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}} - \kappa_2 \rho^{\alpha} \right) \cdot \left| \dot{\gamma}^{\alpha} \right|$$ (Kocks, 1976)

Single Crystal CP-FEM Predictions



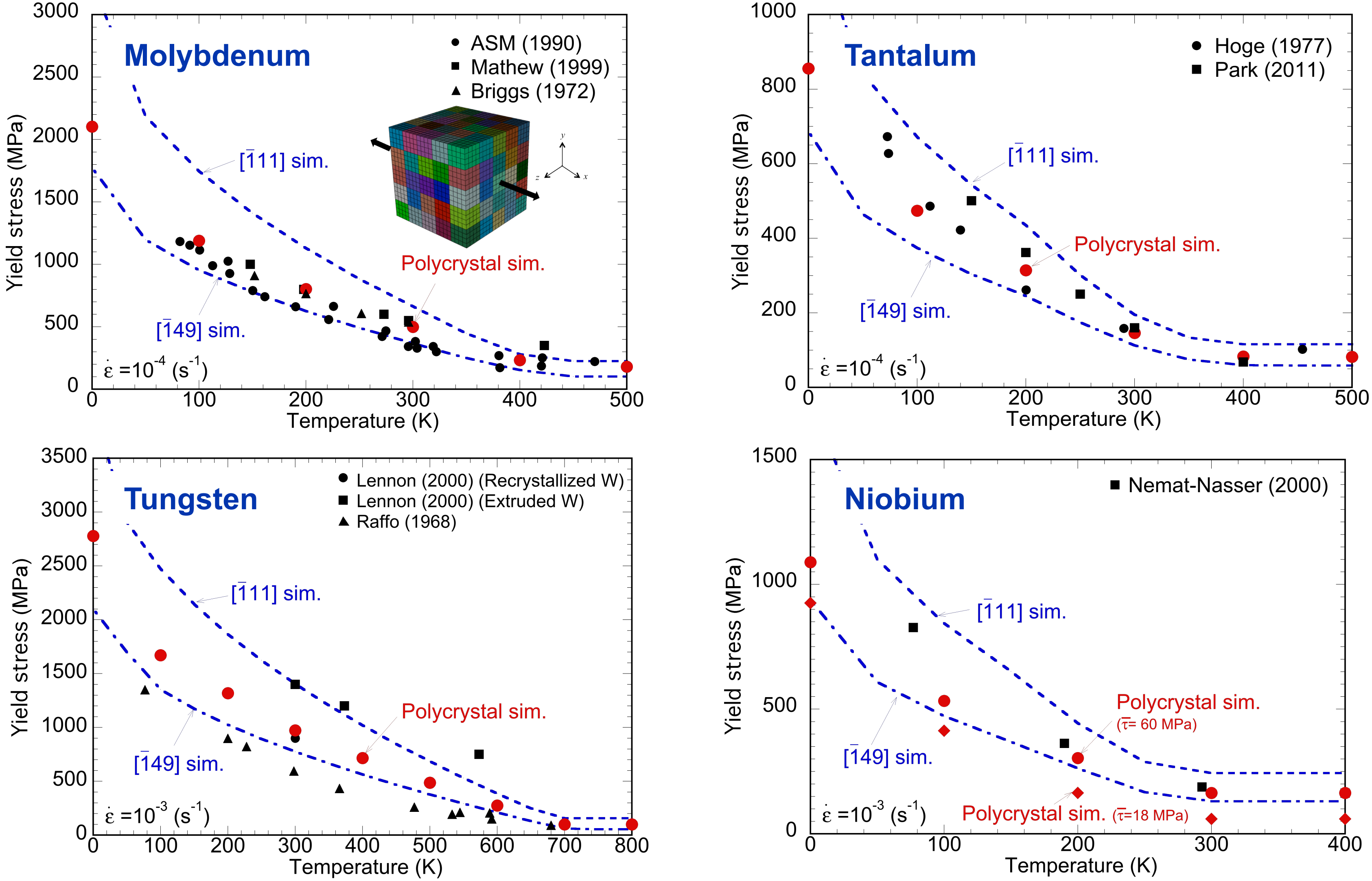






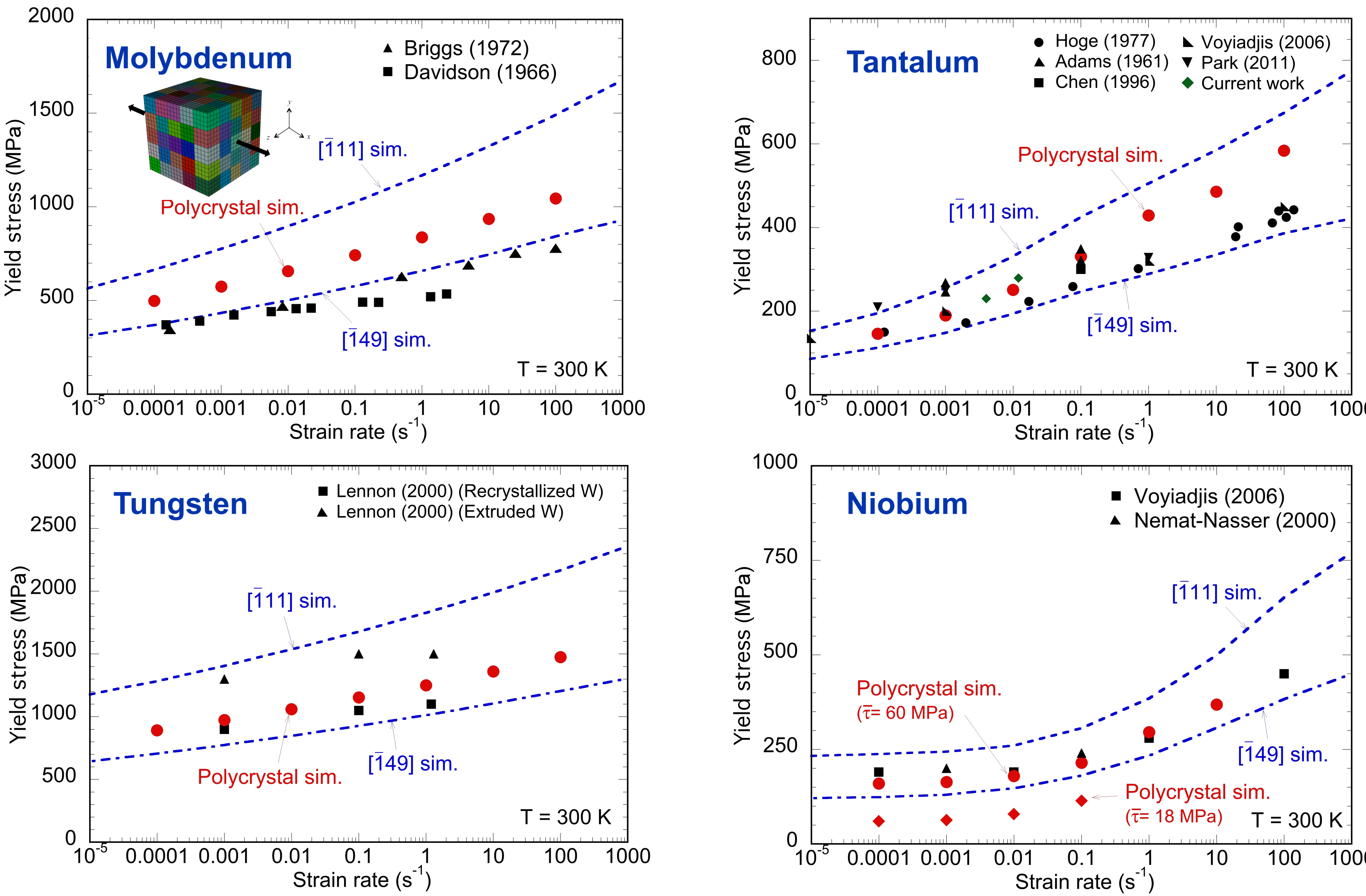
CP-FEM model accurately reproduced yield stresses of [$\bar{1}$49] single crystals

BCC Polycrystals: Temperature Dependence



Measured yield stresses of BCC polycrystals lie between the bounds predicted by CP-FEM models on extreme single crystal orientation.

BCC polycrystals: Strain Rate Dependence



Measured yield stresses of BCC polycrystals lie between the bounds predicted by CP-FEM models on extreme single crystal orientation.

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Continuum-Scale Polycrystal Models

- Johnson and Cook (JC) model (Johnson and Cook, 1983, 1985)

$$\sigma_y^{JC} = A\left(1 + C\ln\dot{\varepsilon}\right)\left(1 - T^{*m}\right)$$

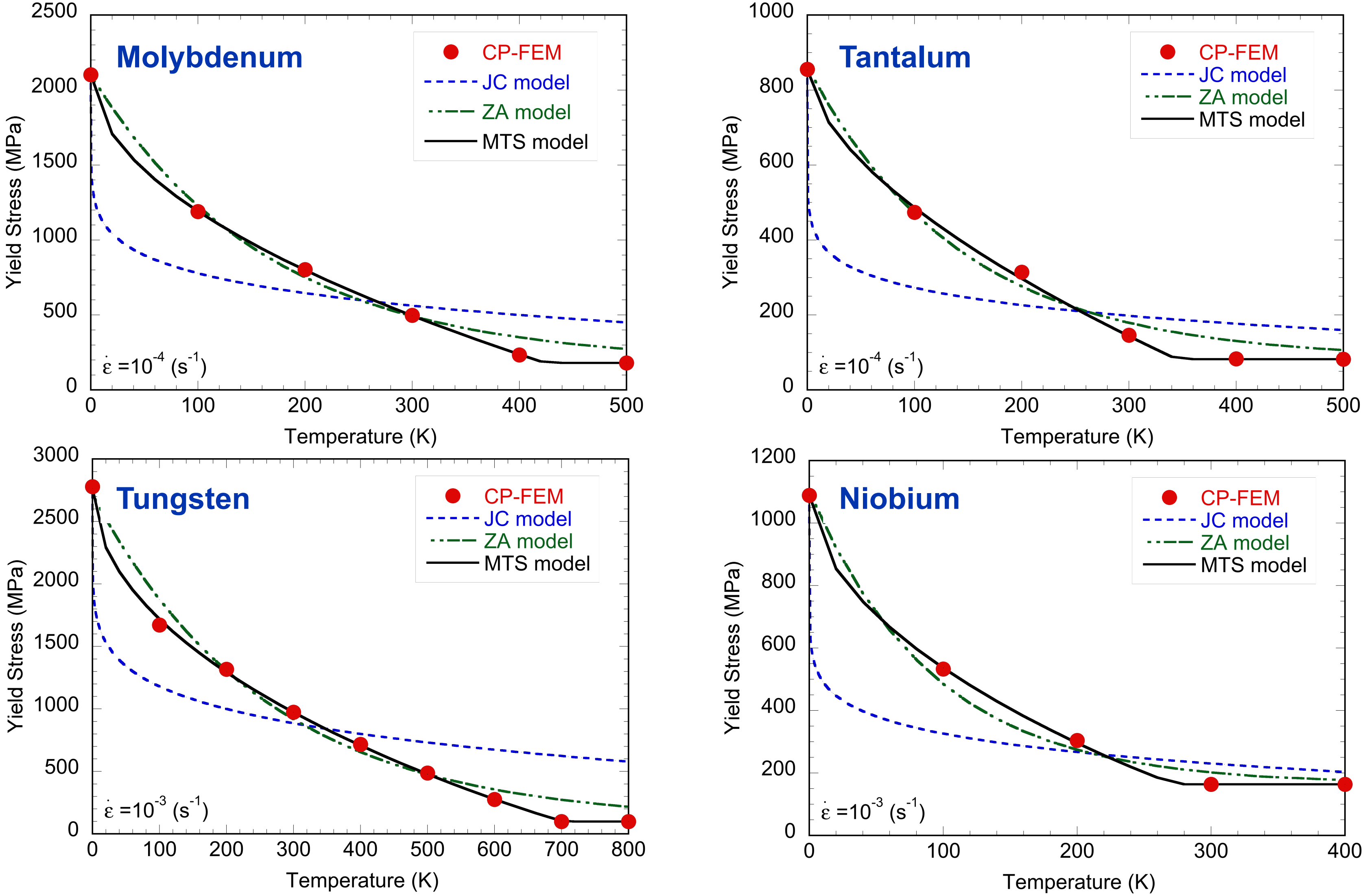
- Zerilli-Armstrong (ZA) model (Zerilli and Armstrong, 1987)

$$\sigma_y^{ZA} = C_0 + C_1\exp\left(-C_3T + C_4T\ln\dot{\varepsilon}\right)$$

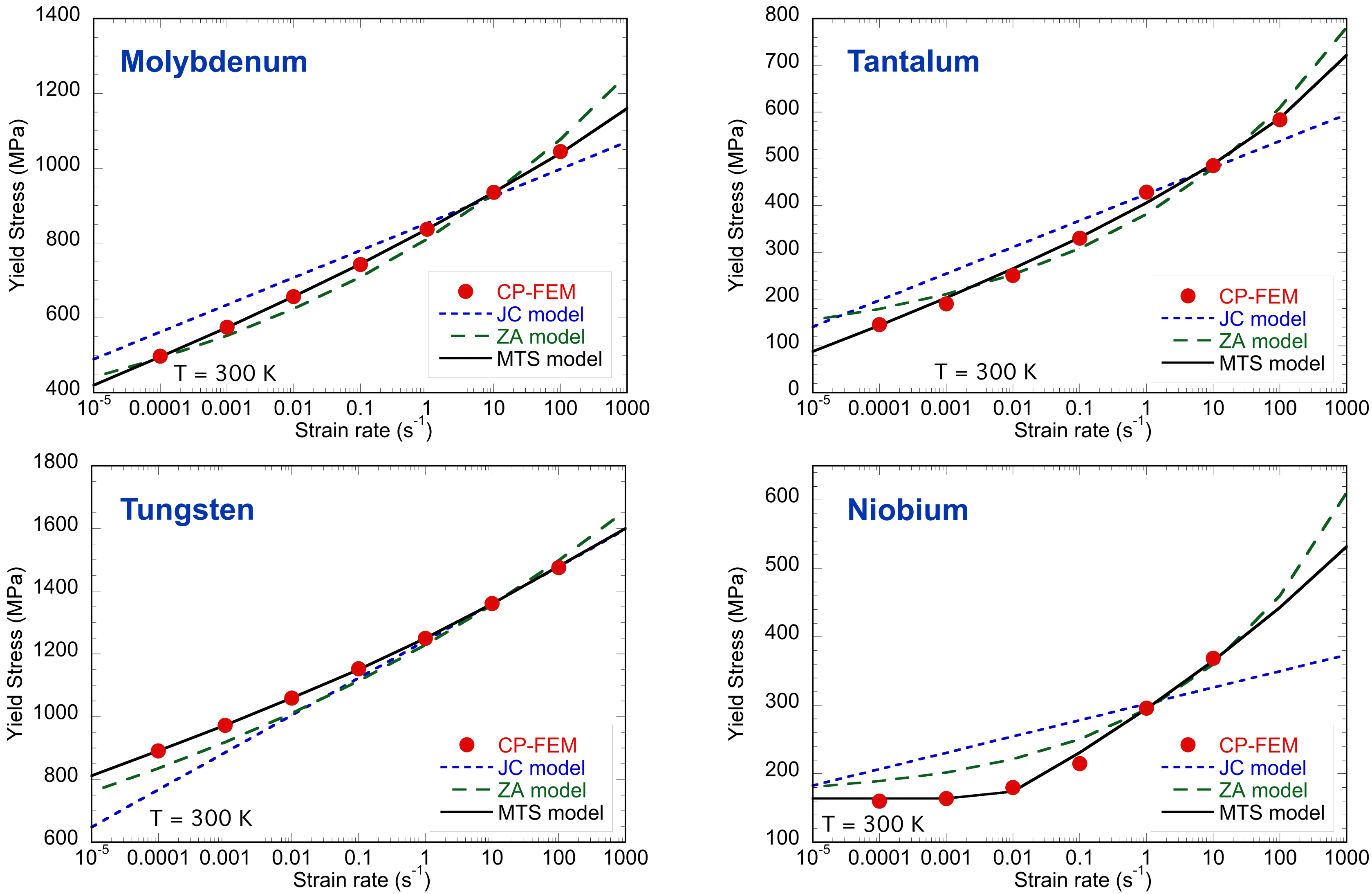
- Mechanical Threshold Stress (MTS) model (Follansbee, 1988)

$$\sigma_y^{MTS} = \sigma_0 + \hat{\sigma}\left(1 - \left(\frac{k_B T}{G_0}\ln\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)^{1/q}\right)^{1/p}$$

Polycrystal Fitting: T dependence



Polycrystal Fitting: Rate dependence



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Polycrystal Fitting: Summary

- JC model: $\sigma_y^{JC} = A(1 + C \ln \dot{\varepsilon})(1 - T^{*m})$
- ZA model: $\sigma_y^{ZA} = C_0 + C_1 \exp(-C_3 T + C_4 T \ln \dot{\varepsilon})$
- MTS model: $\sigma_y^{MTS} = \sigma_0 + \hat{\sigma}\left(1 - \left(\frac{k_B T}{G_0} \ln \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)^{1/q}\right)^{1/p}$

Standard deviations of yield stresses between CP-FEM predictions and continuum fits (unit: MPa)

	JC model	ZA model	MTS model
Mo	165.4	48.9	**2.1**
Ta	78.3	28.2	**10.2**
W	242.1	82.0	**14.2**
Nb	78.7	30.4	**6.0**
Avg.	141.1	47.4	**8.1**

MTS model most accurately reproduce temp./ rate dependent polycrystalline behavior

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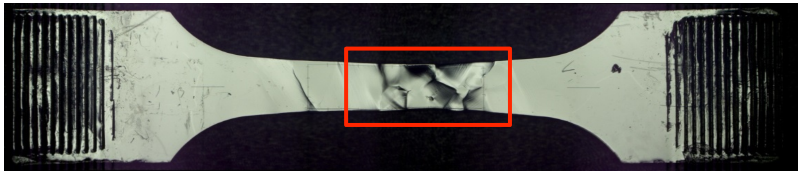
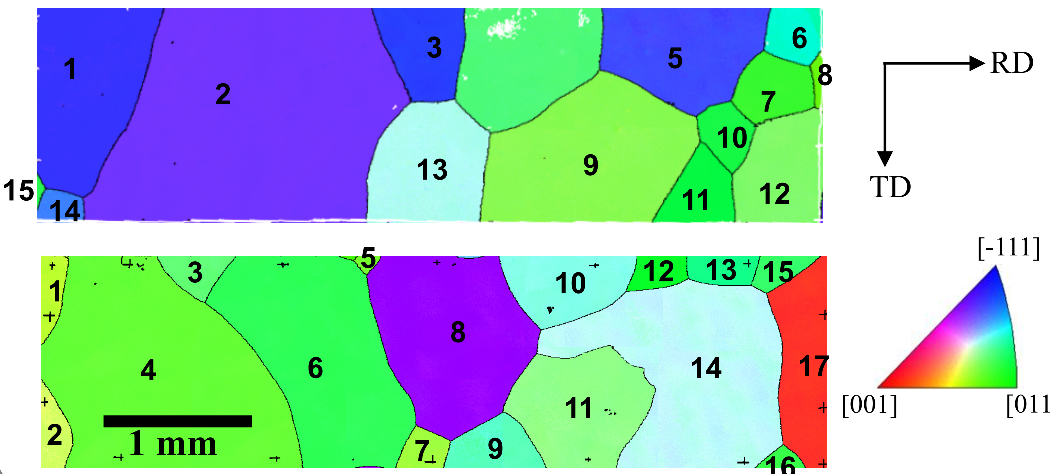
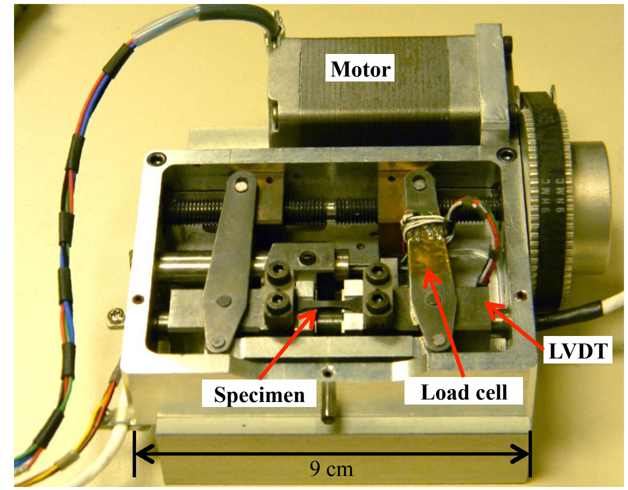
Simulation of Tantalum Oligocrystals

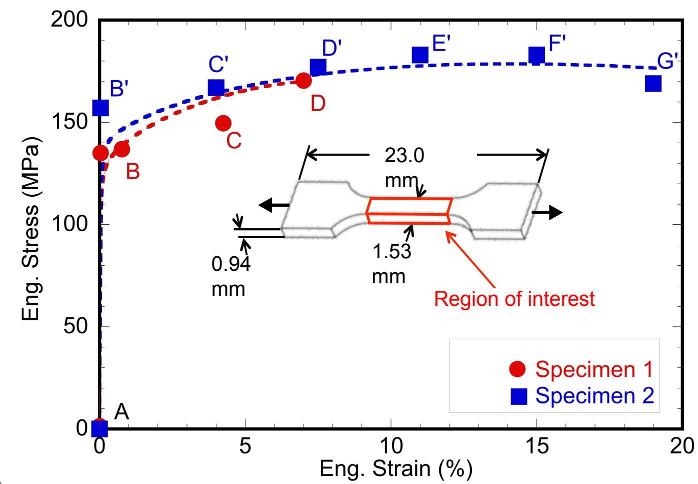
Initial grain orientations



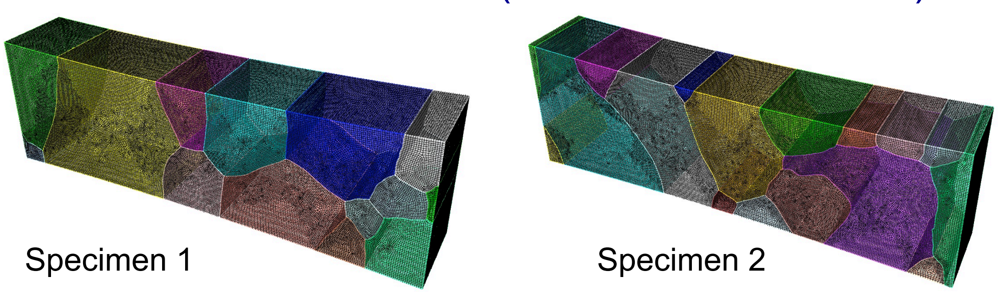


In-situ tensile test inside SEM

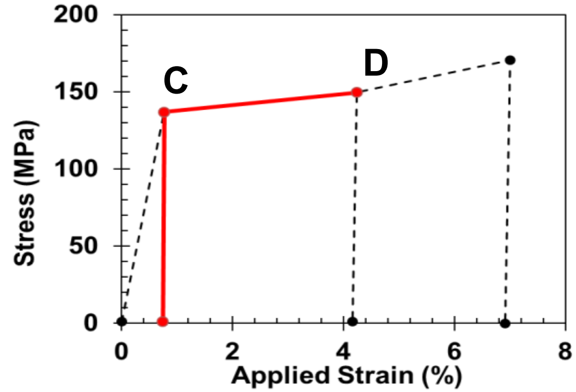




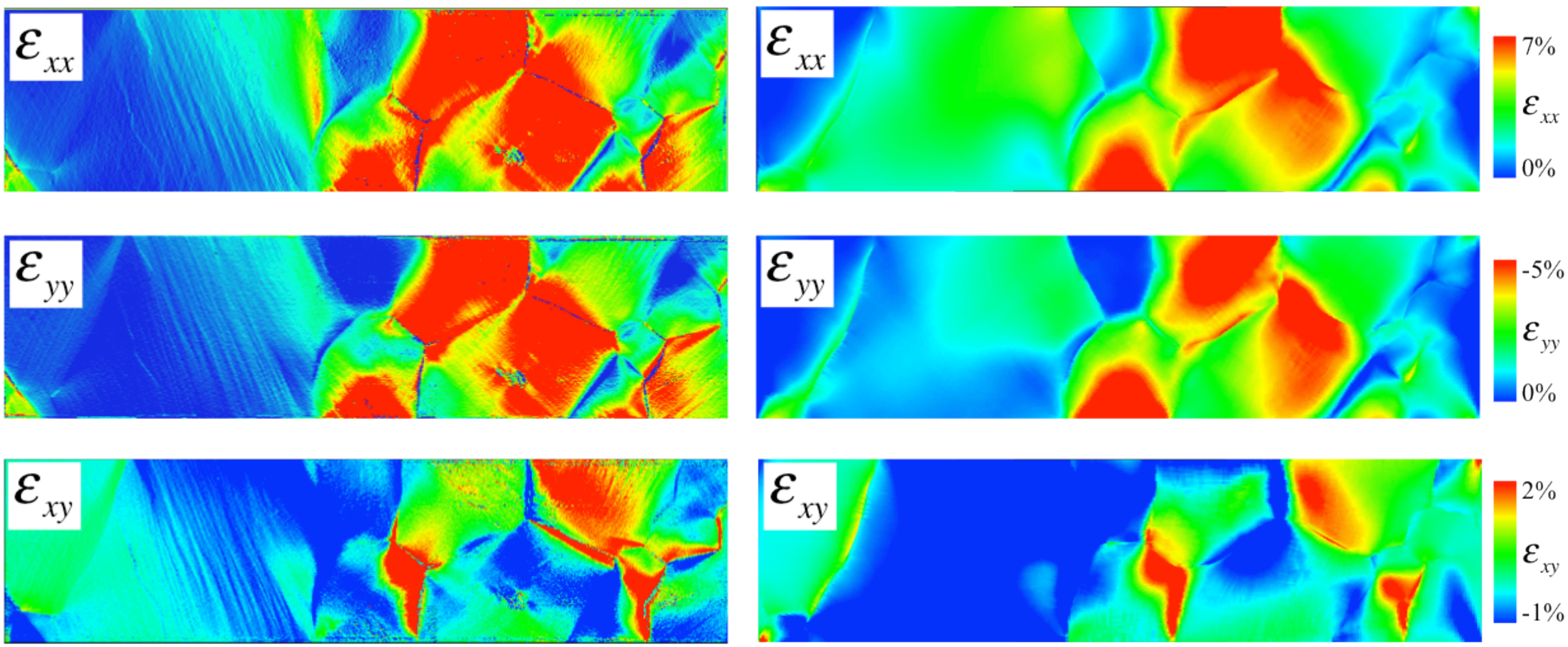
Finite element meshes (~1.5 million elements)



Strain Field Analysis



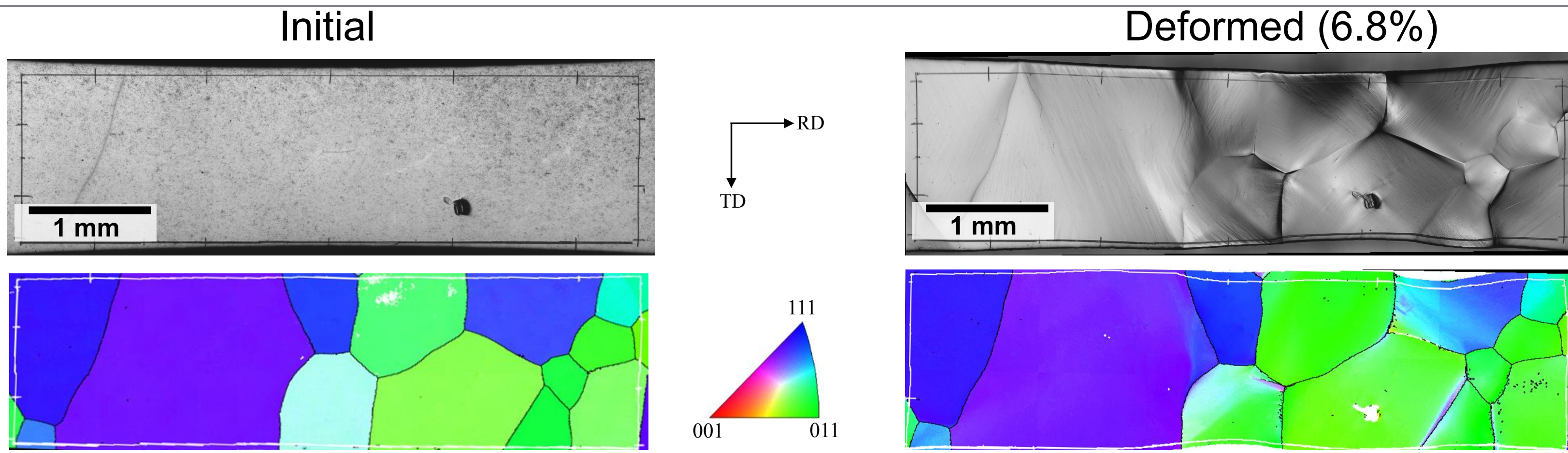
$\Delta\varepsilon_{CD}$ =3.4%

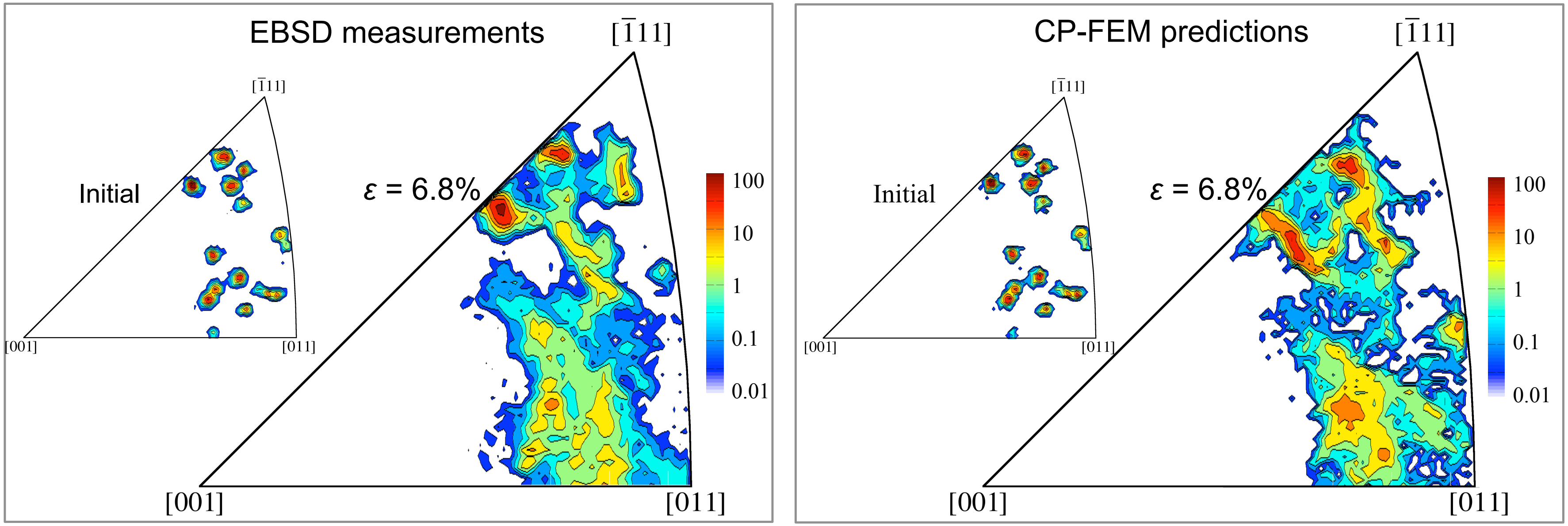


(a) HR-DIC measurements (b) CP-FEM predictions

Measured and predicted strain fields agree well quantitatively.

Texture Analysis

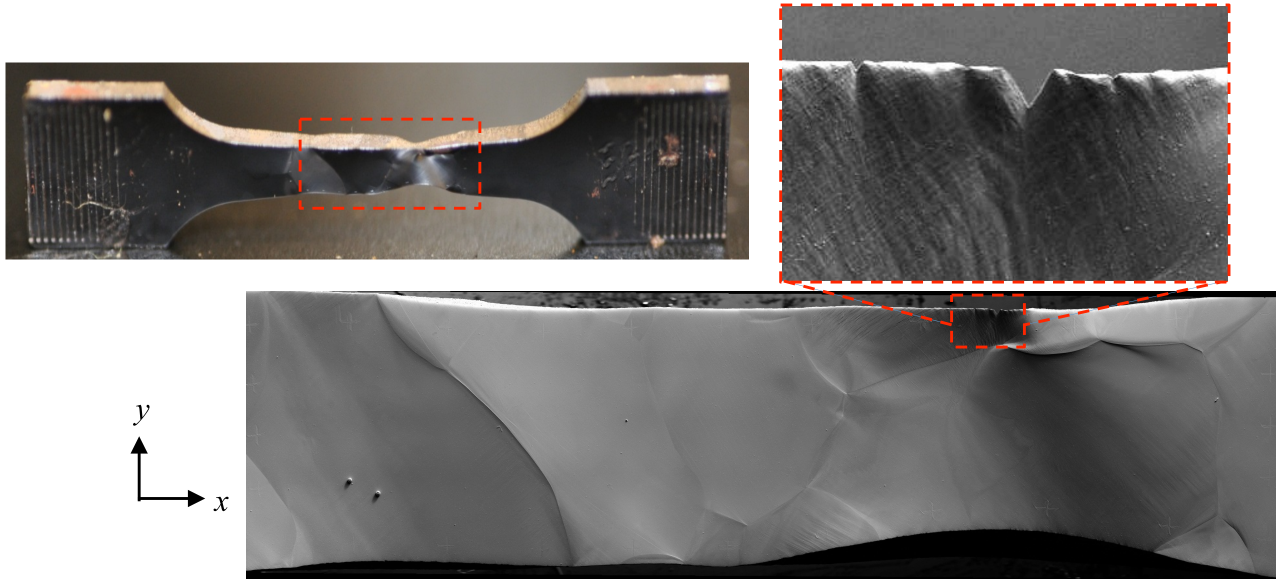




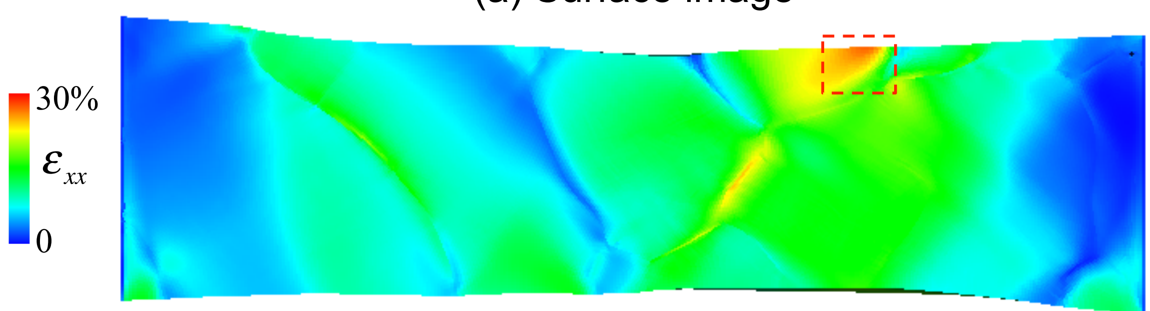
Measured and predicted texture (ε =6.8%)

Prediction of Failure Location

Ta oligocrystal specimen 2 at 19.2% deformation



(a) Surface image



(b) Simulated ε_{xx}

Failure location agrees with the location of the highest ε_{xx} from the simulation

Summary

- Developed T and $\dot{\varepsilon}$ dependent flow rule based on dislocation kink-pair theory for Mo, Ta, W and Nb.
- Predicted T and $\dot{\varepsilon}$ dependent σ_y using CP-FEM model agree well with experimental data.
- MTS model accurately reproduced polycrystal behavior.
- CP-FEM predictions of Ta oligocrystals showed good agreement with measured strain fields (HR-DIC) and deformed textures (EBSD).
- Proposed computational method provides a convenient and direct link from the fundamental dislocation physics to the continuum-scale plastic deformation of BCC metals at the grain scale.

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THANK YOU !

Email: hnlim@sandia.gov