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# Dislocation kink-pair theory as a basis for temperature- and rate-dependent BCC crystal plasticity model

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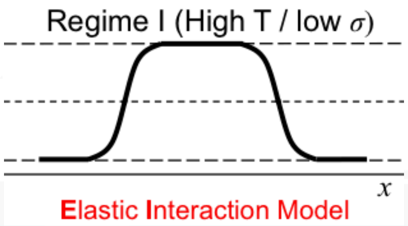
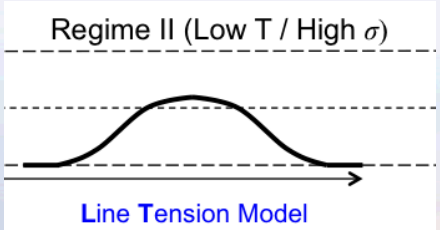
# Multi-Scale Modeling of BCC Plasticity

**Atomic Scale** | **Crystal Plasticity** | **Microstructure** | **Macro-Scale**

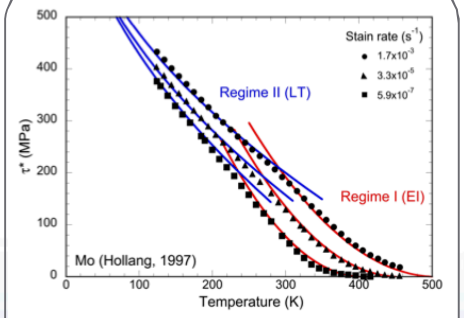


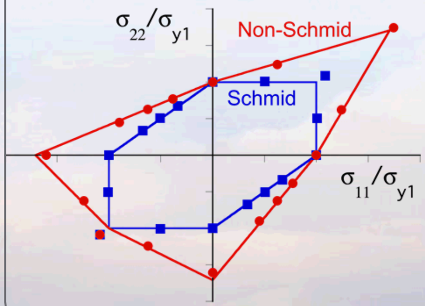
Elastic Interaction Model



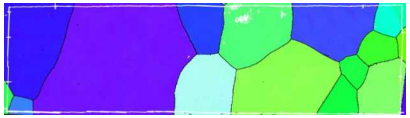
Line Tension Model

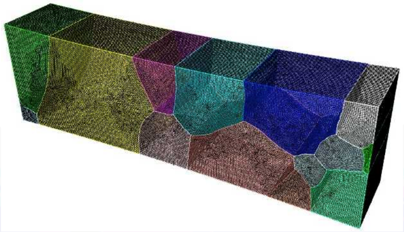
Dislocation Physics



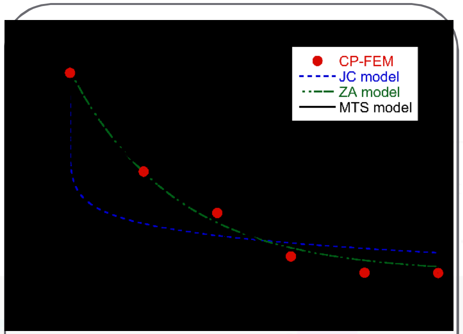


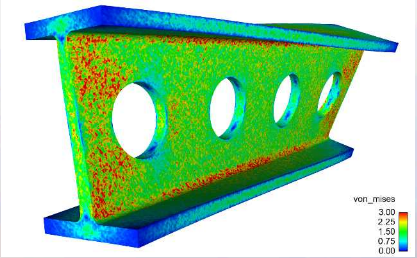
Single Crystal Behavior





Polycrystal Properties



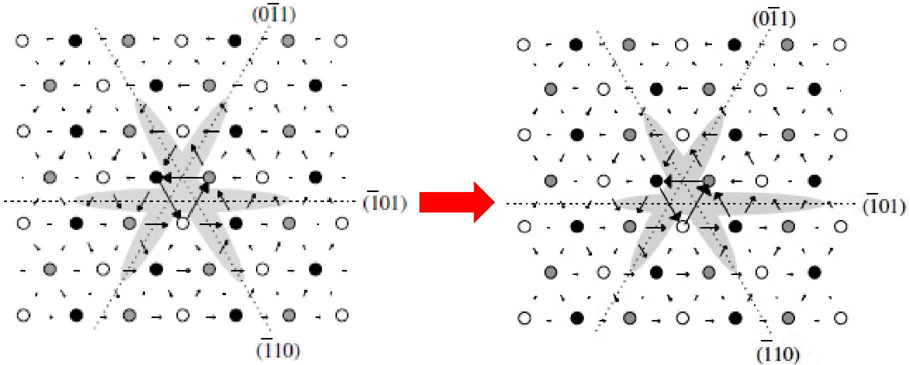


Macroscale Models

# Nano: Atomic Properties of Dislocations in BCC Metals

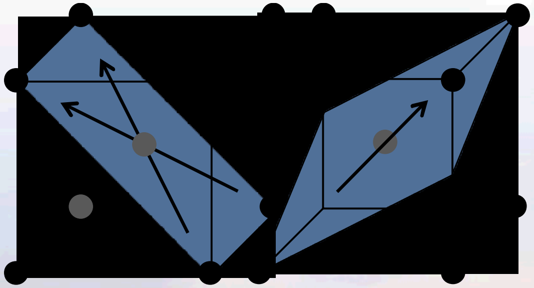
## Screw dislocations in BCC metals have complex atomic structures …

[111] zone depiction of a relaxed **screw** dislocation core in Mo



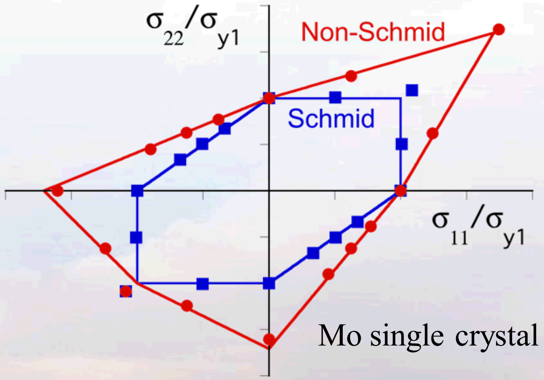
Distortion of the dislocation core under an applied shear stress

Groger, Vitek et al. *Acta Mat.* 56 (2008) 5412.

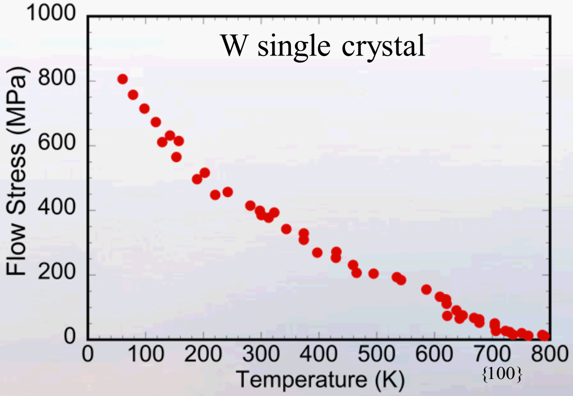


{110} slip + {112} slip
( + {123} slip? )

Uncertainty about important slip systems



Non-Schmid plasticity

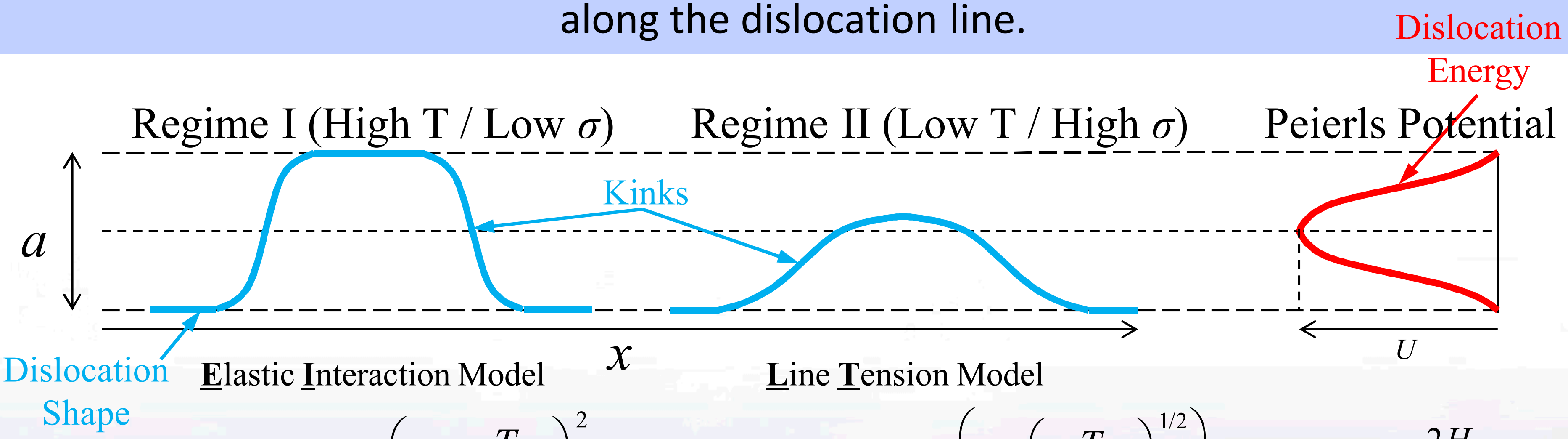


Strong temperature and strain rate sensitivity

… and this leads to various non-ideal behaviors and properties.

# Dislocation Kink-Pair Theory

Dislocation motion occurs by the formation and propagation of atomic-scale kinks along the dislocation line.



**E**lastic **I**nteraction Model

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

**L**ine **T**ension Model

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

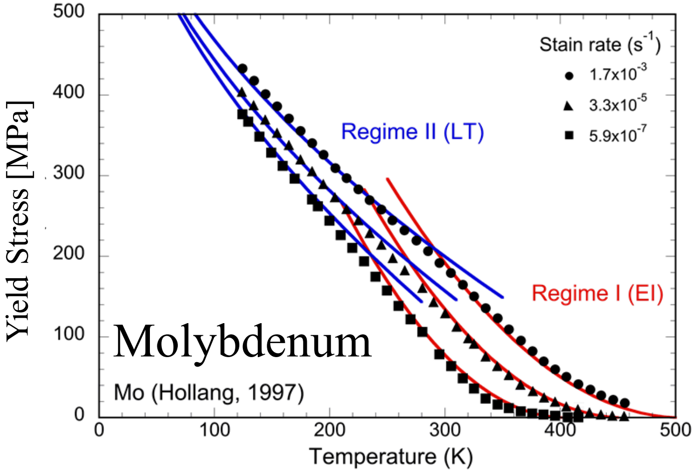
(Antiparabolic Peierls potential)

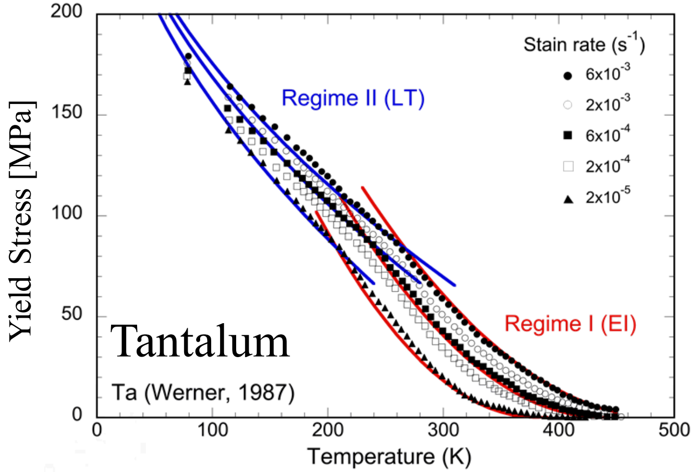
$$T_c(\dot{\gamma}) = \frac{2H_k}{k_B \ln\left(\dot{\gamma}_0/\dot{\gamma}\right)}$$

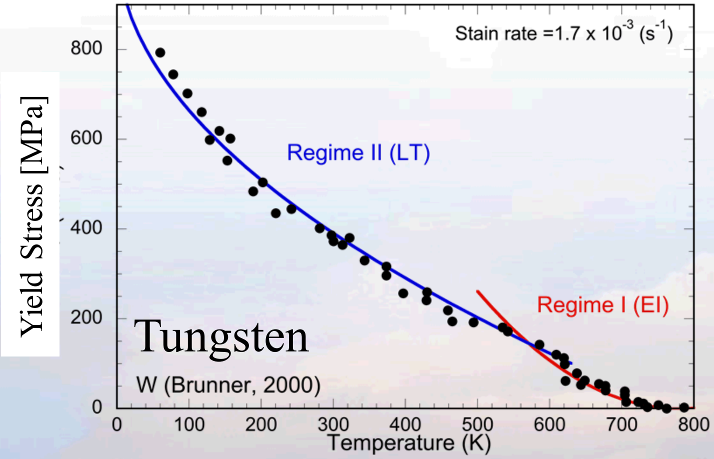
The atomic-scale properties of BCC screw dislocations guide the development of a dislocation kink-pair model for how the temperature and strain-rate affect a BCC metal's yield stress.

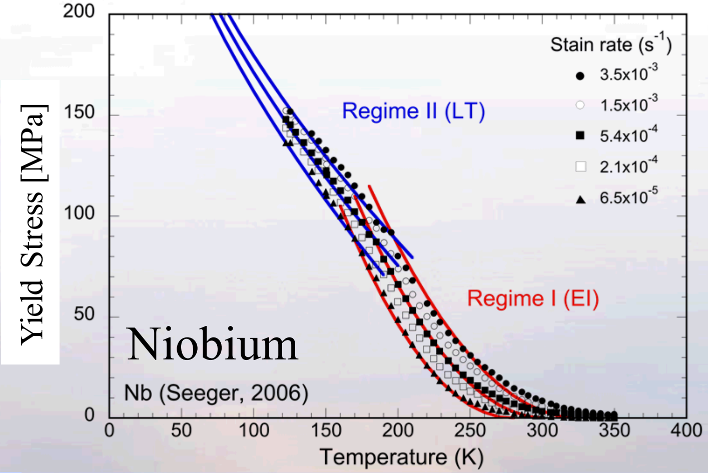
Seeger, Z. Metallk. 1981
Seeger, Mater. Sci. Eng. A, 2001
Butt, Phil. Mag. 2007
Argon, Strengthening mechanisms in crystal plasticity 2008

# Confirming the form of the “Kink-Pair” Model and calibrating to single crystal data







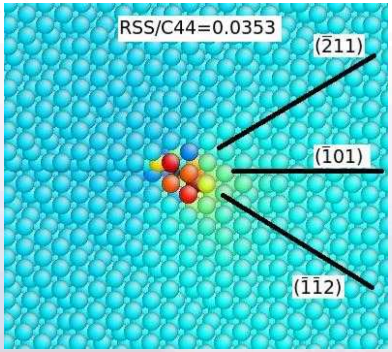


Our dislocation kink-pair model accurately reproduces experimental data for the yield stress over a range of BCC metals, temperatures, and strain rates.

# 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,…)**

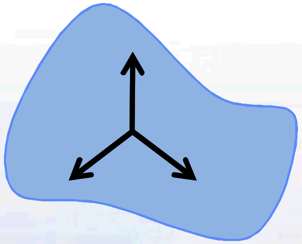
Atomic phenomenology:
Fundamental deformation
mechanisms



Yield criterion

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

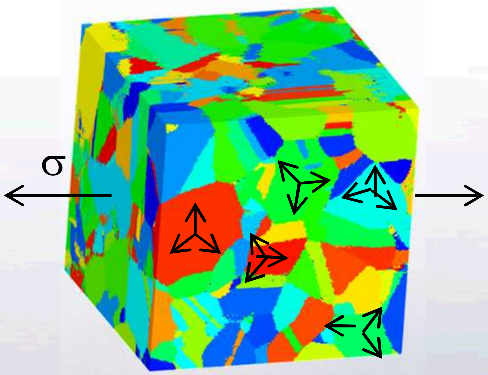
Single crystal
plasticity:
Deformation of one,
isolated crystal



Constitutive law

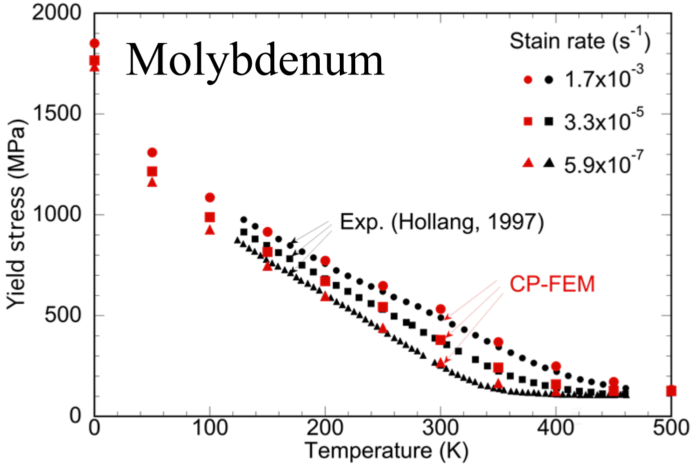
$$\dot{\gamma}^{(s)} = \frac{\tau^{(s)}}{\tau_{cr}}\left|\frac{\tau^{(s)}}{\tau_{cr}}\right|^{\frac{1}{m}-1}$$

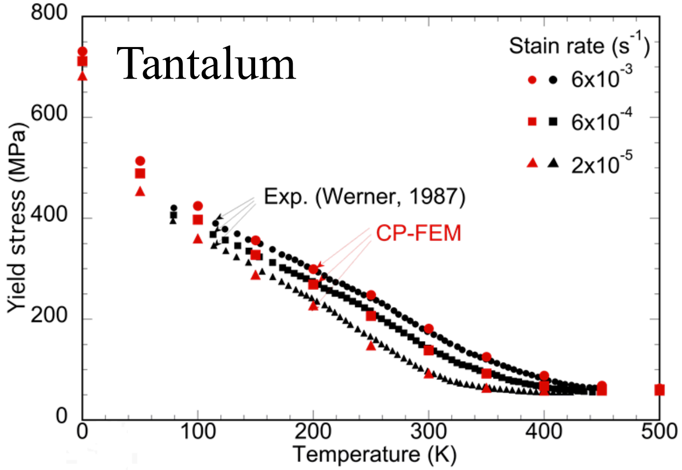
Polycrystal plasticity:
Assemble single crystals into
polycrystalline ensemble

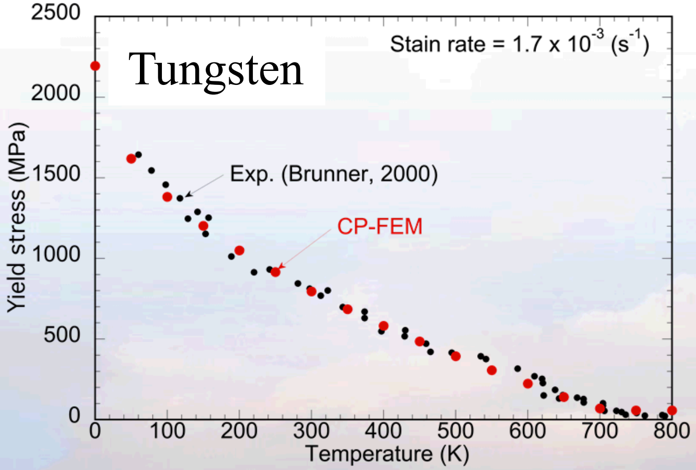


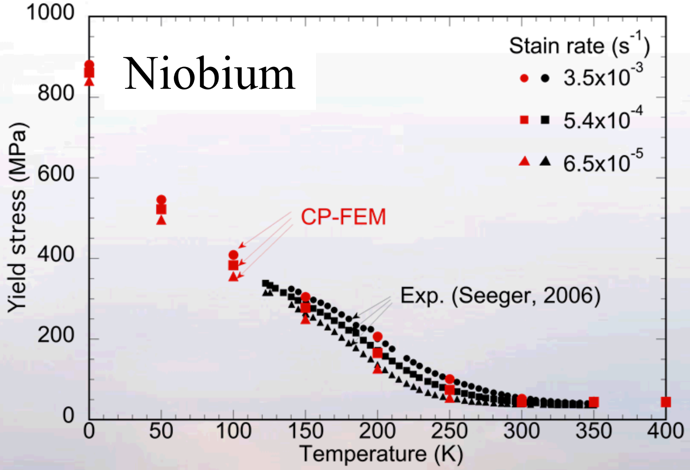
Prediction of collective deformation behavior

# Micro: Implementation into Single-Crystal Plasticity



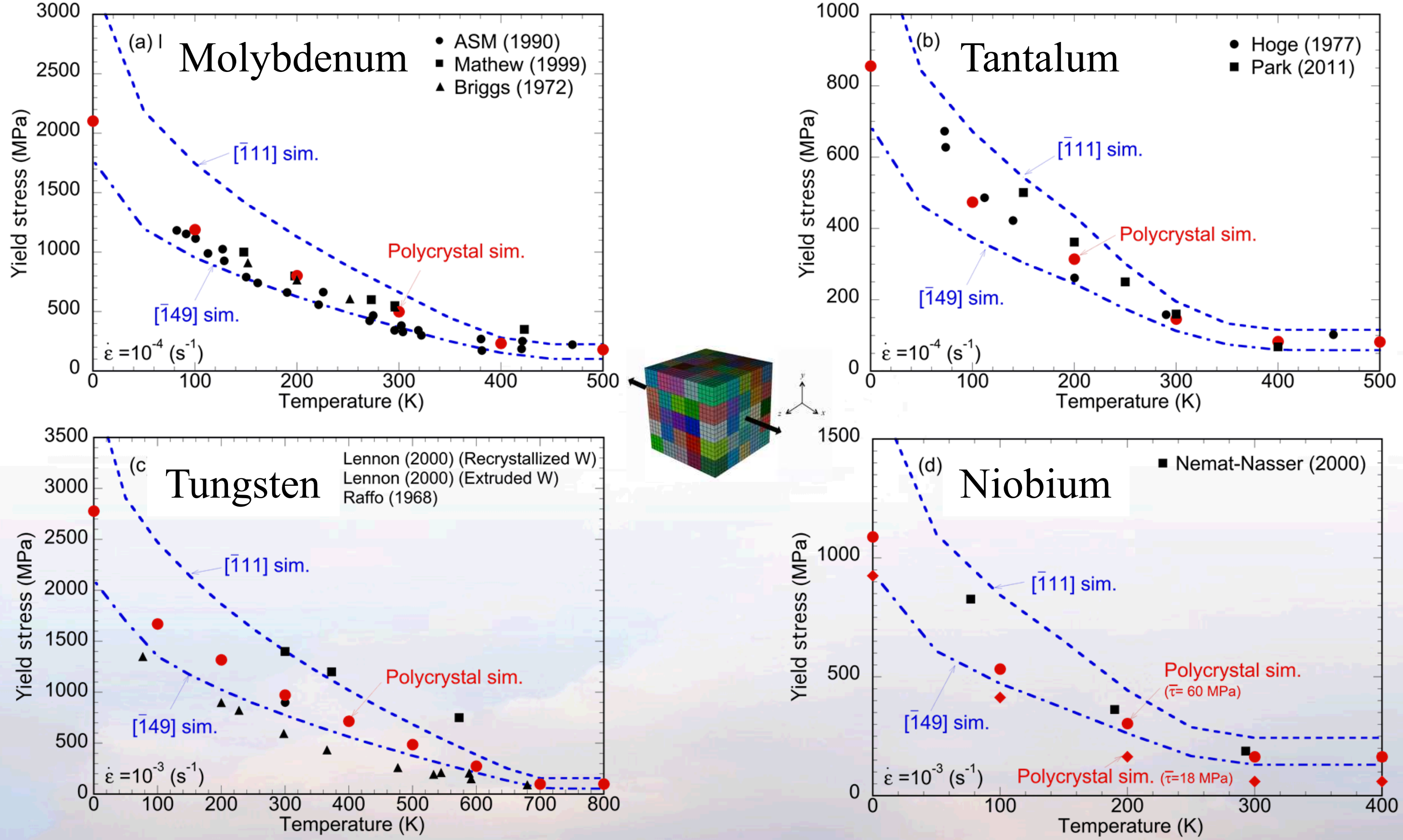






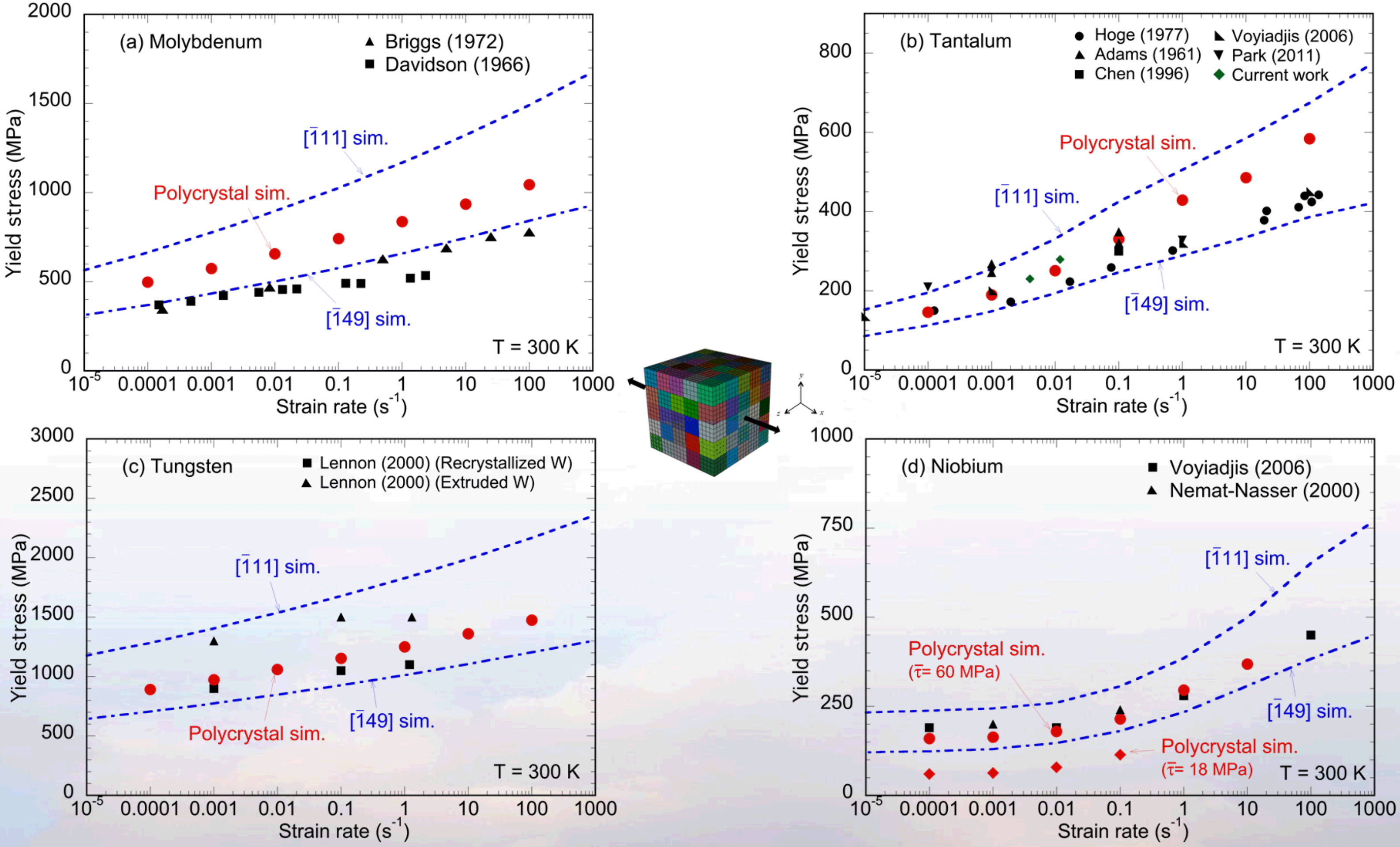
Moving up in scale and implementing the theory into a crystal plasticity finite element model (CP-FEM) for single-crystal BCC plasticity, the quality of validation is retained.

# Meso: Up-Scaling into Polycrystal Plasticity



The next length scale is the polycrystal, where CP-FEM simulations agree very well with experiments, even when calibrated only to independent, single-crystal tests.

# Meso: Up-Scaling into Polycrystal Plasticity



Moving up again in scale, CP-FEM simulations agree very well with experiments, even when using only calibrations to independent, single-crystal tests.

# Macro: Classical Continuum 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)

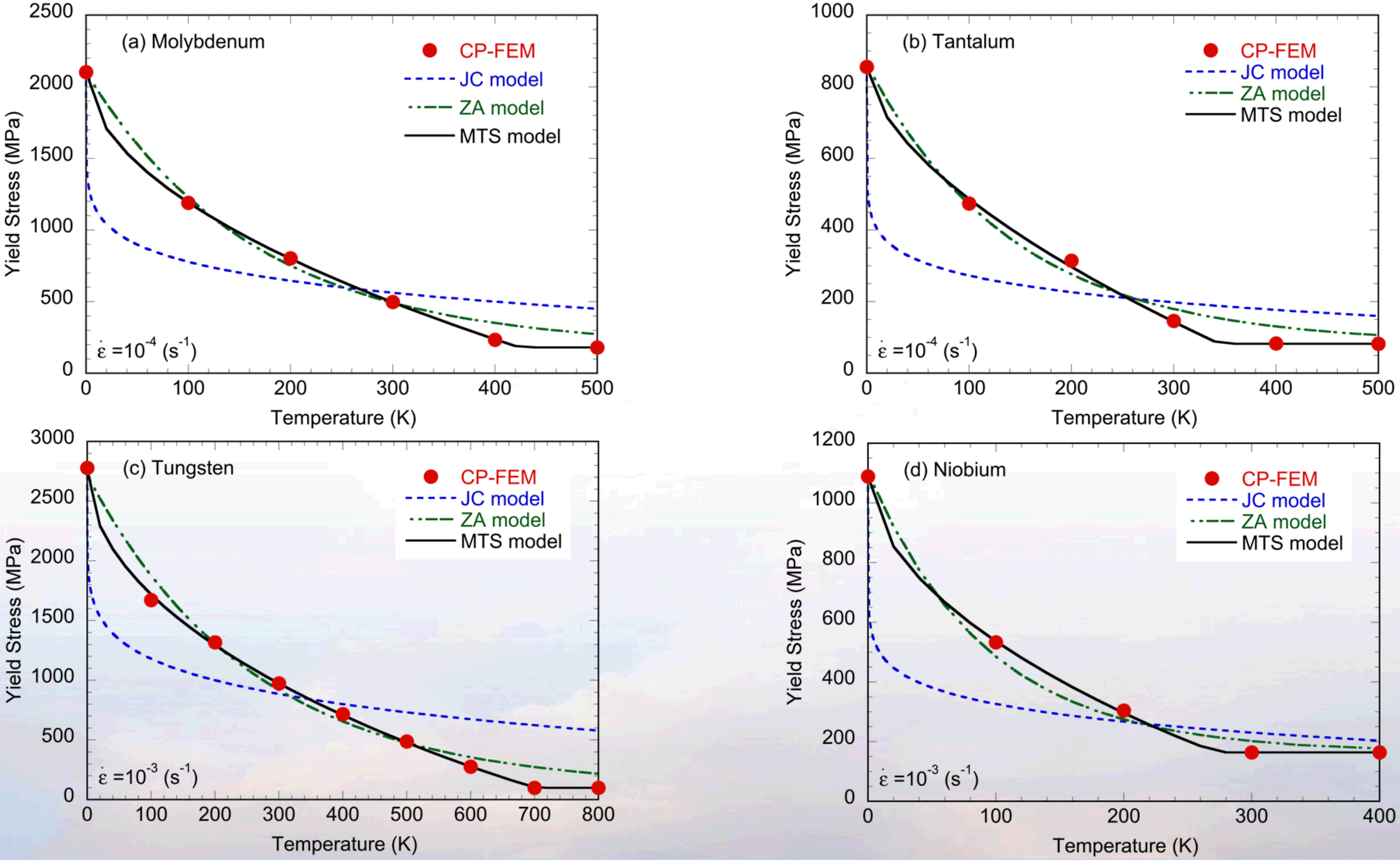
$$\sigma_y^{ZA} = C_0 + C_1\exp\left(-C_3T + C_4T\ln\dot{\varepsilon}\right)$$

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

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

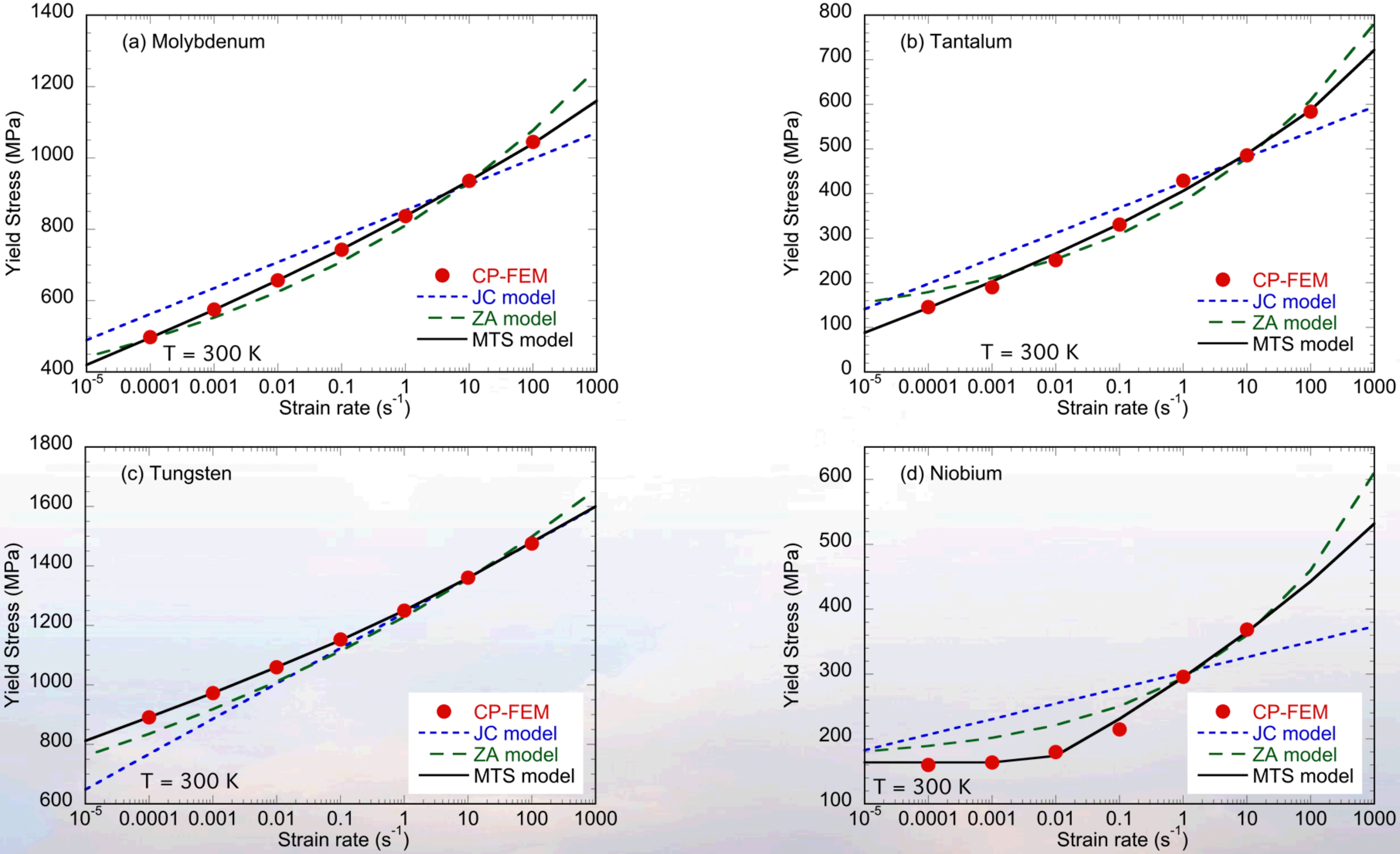
Sandia's macro-scale engineering analysis codes use conventional constitutive models to describe temperature and strain-rate effects.

# Macro: Interfacing CP-FEM into Continuum Models



Our CP-FEM simulations, derived from atomic-scale considerations of BCC dislocations, provide a direct link to these continuum models' parameters.

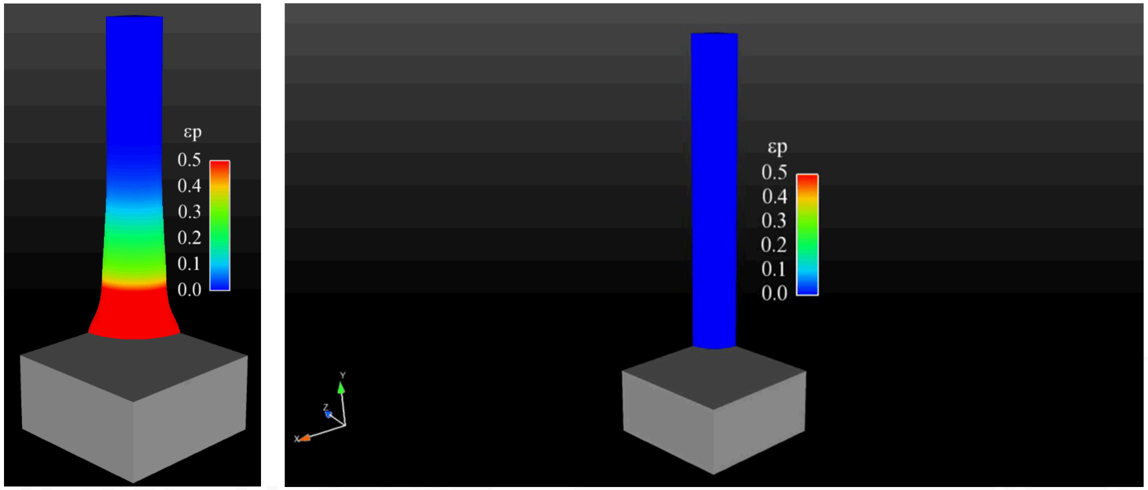
# Macro: Interfacing CP-FEM into Continuum Models



Our CP-FEM simulations, derived from atomic-scale considerations of BCC dislocations, provide a direct link to these continuum models' parameters.

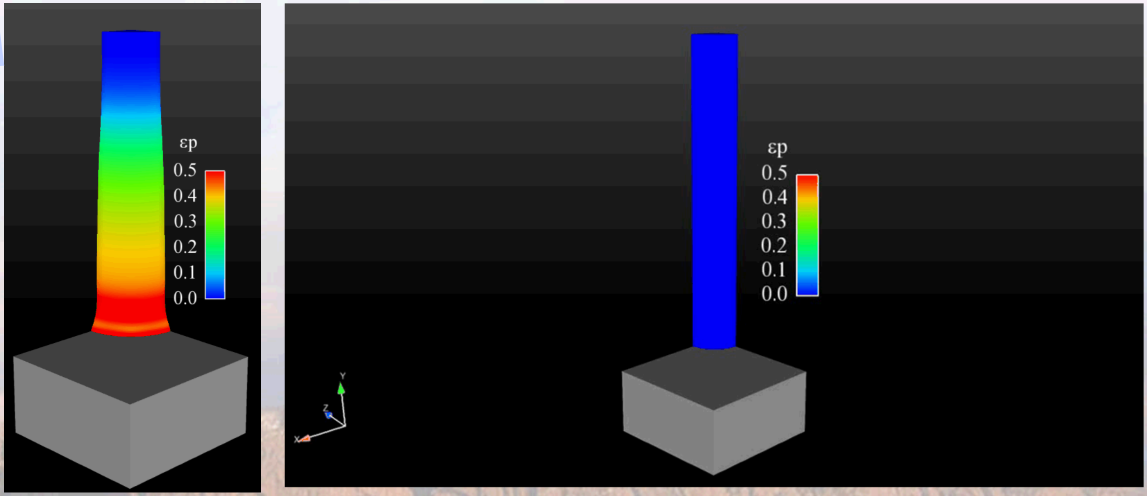
# What’s next: From Atomic-Scale Dislocation Theory into Alegra (Sandia parallelized continuum dynamics code)

Johnson-Cook



We are ramping up parameterizations of JC, ZA, MTS, and BCJ for use in codes such as Alegra and CTH

Zerilli-Armstrong



# Summary

1. Existing dislocation kink-pair theory forms a basis for understanding how the peierls barrier manifests in temperature and rate-dependence
2. This theory provides single crystal flow rules that are now embedded in a polycrystal plasticity framework
3. The single crystal flow rules can be calibrated on existing single crystal literature data; the 4-parameter model form fits exceptionally well.
4. Within the crystal plasticity model, the form of the temperature and rate dependence matches experimental polycrystal data.
5. At the macro-scale, this kink-pair based crystal plasticity model compares very favorably with the MTS model for temperature strain-rate dependence.

Lim, Battaile, Carroll, Weinberger, Boyce, "A physically based temperature and strain rate dependent crystal plasticity model for BCC metals," *J. Mechanics and Physics of Solids*, 2014.