KEYNOTE LECTURE

Atomistic Simulations of Dislocation Nucleation

M.A. Tschopp [1,2], D.L. McDowell [3,4]

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[4]GWW School of Mechanical Engineering
Georgia Institute of Technology

12th International Conference on Fracture 2009

Atomistic Fracture & Deformation T03-S5

Thursday, July 16, 2009, 13:50-14:30

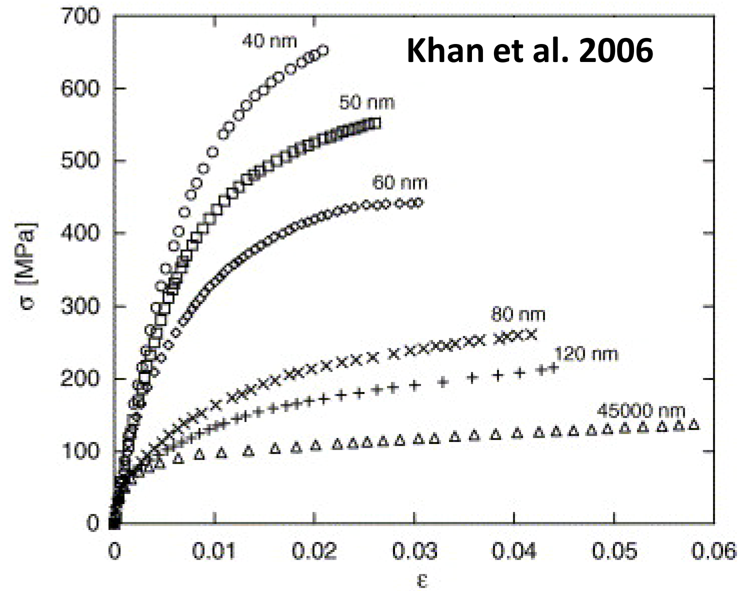
Outline

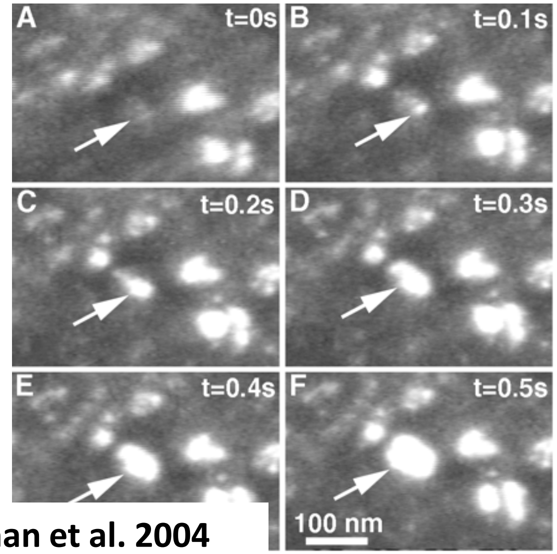
- **Introduction**
- **Simulation Methodology**
- **Bicrystal Atomistic Simulations Results**
  - Grain Boundary Characterization
  - Grain Boundary Dislocation Nucleation
- **Single Crystal Atomistic Simulations**
  - Orientation dependence of dislocation nucleation
  - Influence of resolved stresses on dislocation nucleation
  - Temperature dependence of dislocation nucleation
- **Conclusions**

Introduction

Enhanced functional properties in materials with nanoscale dimensions

- Nanocrystalline materials!
- Experiments regarding inelastic mechanisms are often difficult to perform
- Plasticity at the nanoscale is dominated by grain boundary behavior, i.e., grain boundary sliding, grain rotation, and dislocation nucleation





Shan et al. 2004

Introduction

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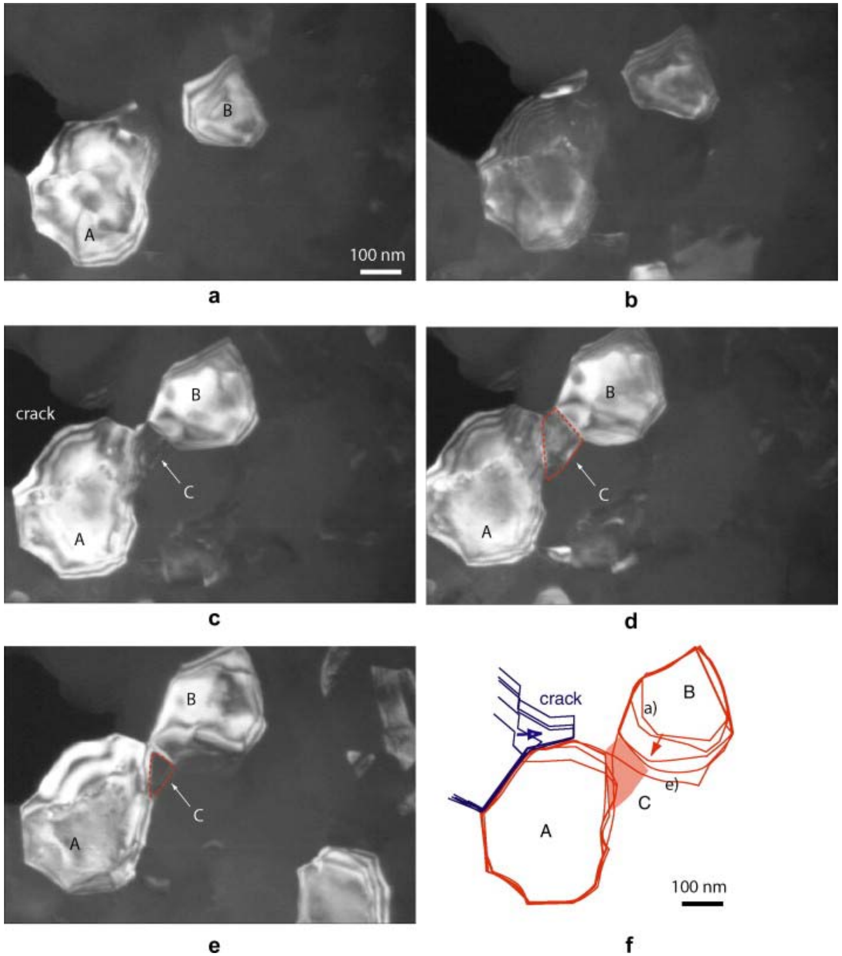
In situ TEM observations of grain-boundary motion in stressed nanocrystalline aluminum films



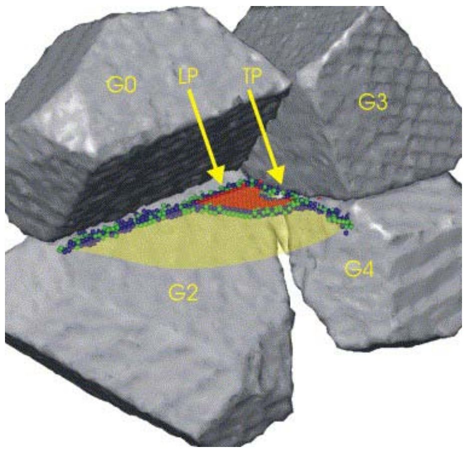
Legros, Gianola, Hemker 2008

Introduction

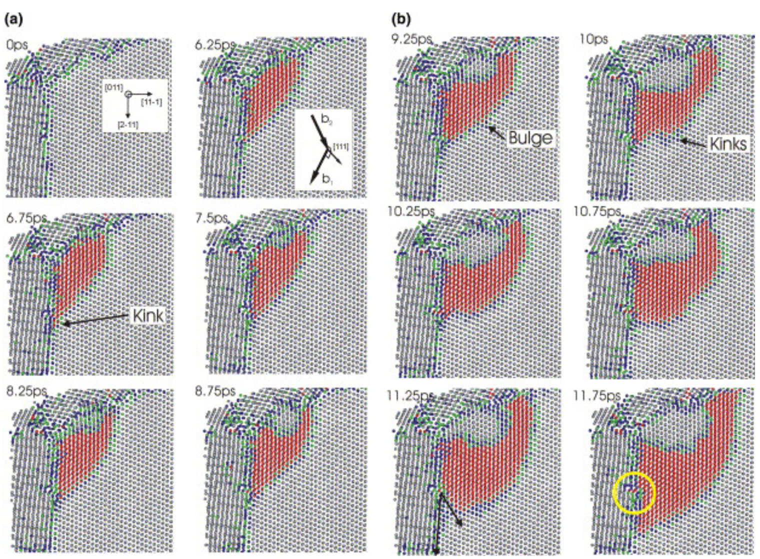
Enhanced functional properties in materials with nanoscale dimensions

Nanocrystalline Atomistic Simulations of Inelasticity at the Nanoscale

- Effective tool for analyzing dislocation nucleation and grain boundary sliding in nanocrystalline materials
- Provides insight into mechanisms and quantitative data that can be used in higher scale models to predict bulk properties of nanomaterials
- Deformation mechanisms agree with limited experimental results



Van Swygenhoven et al. 2006



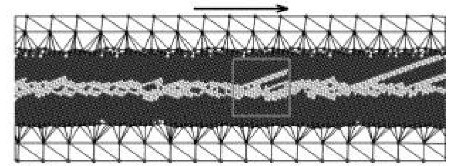
Introduction

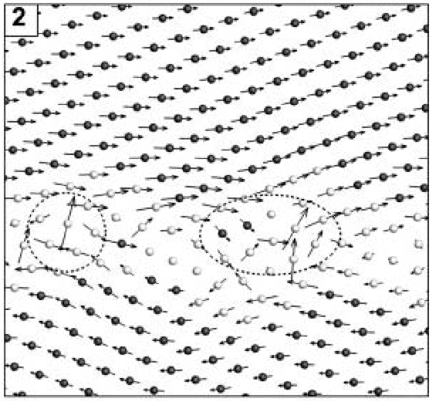
Enhanced functional properties in materials with nanoscale dimensions

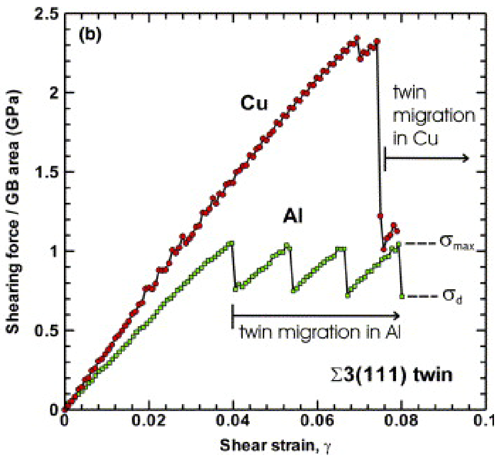
Nanocrystalline Atomistic Simulations of Inelasticity at the Nanoscale

Bicrystal Atomistic Simulations of Inelasticity at the Nanoscale

- Grain boundaries in nanocrystalline materials are very complex, though
- Bicrystal simulations can manipulate grain boundary degrees of freedom to assess their impact on inelastic mechanisms
- Primarily performed on **symmetric** tilt grain boundaries







Sansoz & Molinari 2005; Warner et al. 2006

Introduction

Enhanced functional properties in materials with nanoscale dimensions

Nanocrystalline Atomistic Simulations of Inelasticity at the Nanoscale

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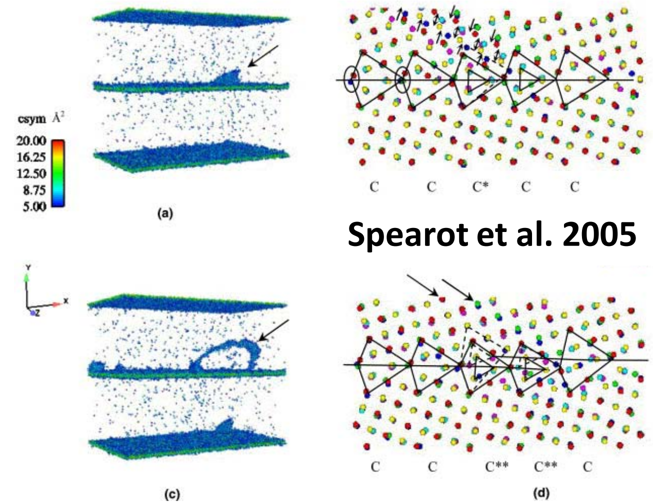
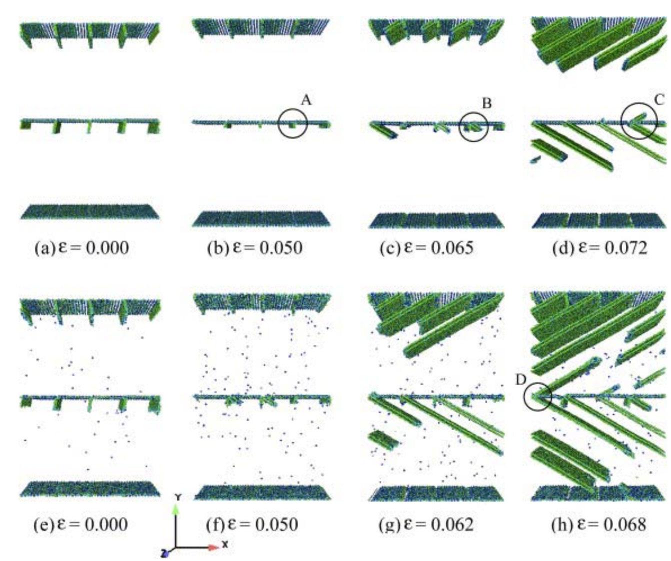


Spearot et al. 2005

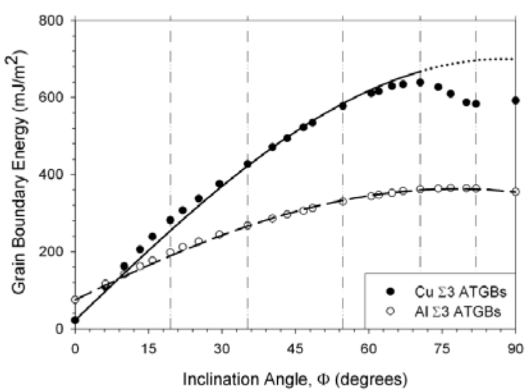


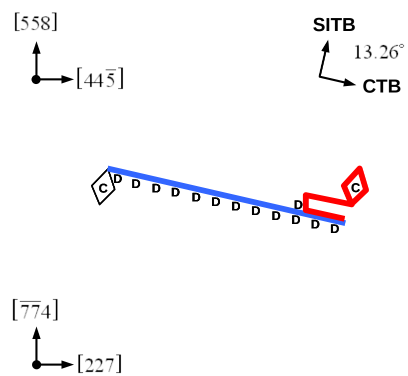
Spearot et al. 2007

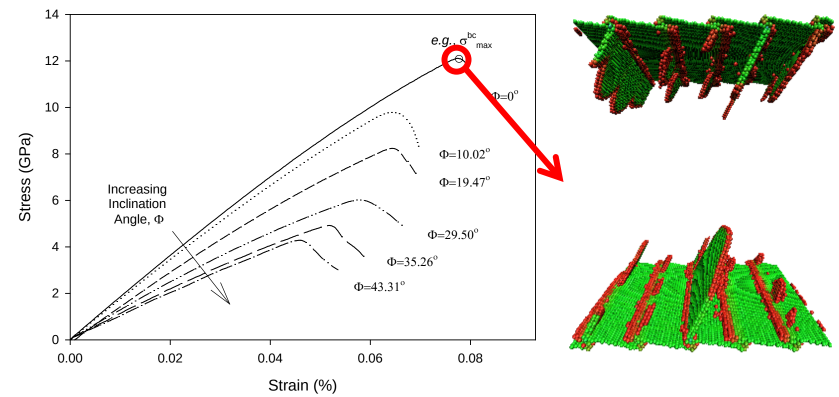
Present research

The present research investigates the influence of grain boundary degrees of freedom on *heterogeneous* dislocation nucleation using ***BICRYSTAL SIMULATIONS***

Energy ⟷ Boundary Structure ⟷ Dislocation Nucleation





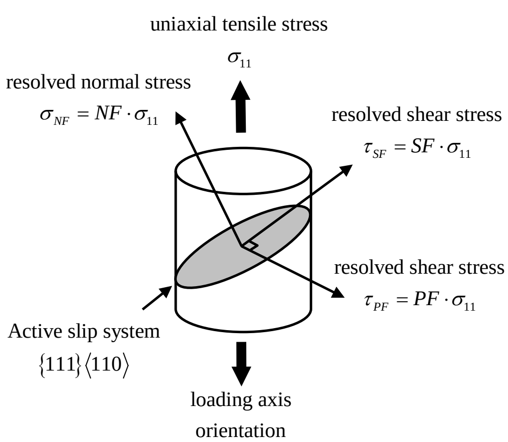


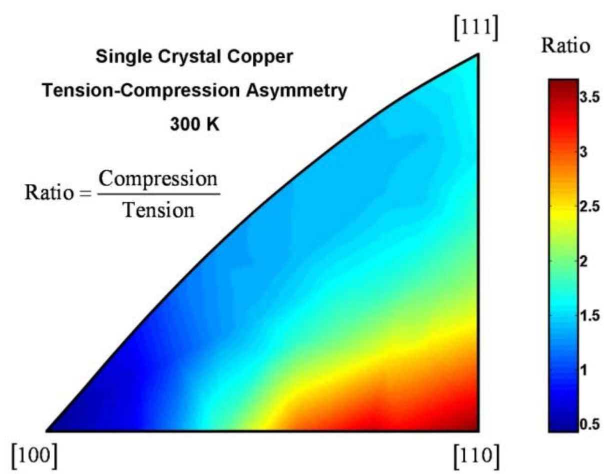
Tschopp, Spearot, McDowell, "Influence of Grain Boundary Structure on Dislocation Nucleation in FCC Metals," Dislocations in Solids, Vol. 14, pp. 43-139 (2008)

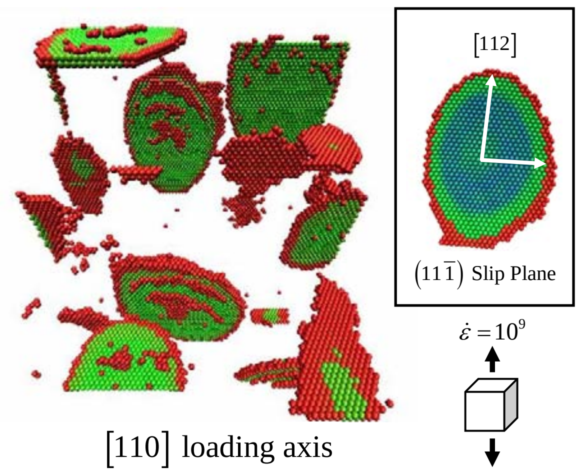
Present research

The present research also investigates *homogeneous* dislocation nucleation for improved understanding of lattice orientation using ***SINGLE CRYSTAL SIMULATIONS***

Resolved Stress ⟷ Lattice Stress Effect ⟷ Dislocation Nucleation







Tschopp, McDowell, "Influence of single crystal orientation on homogeneous dislocation nucleation under uniaxial loading" JMPS 56 (2008) 1806-1830.

Simulation Methodology

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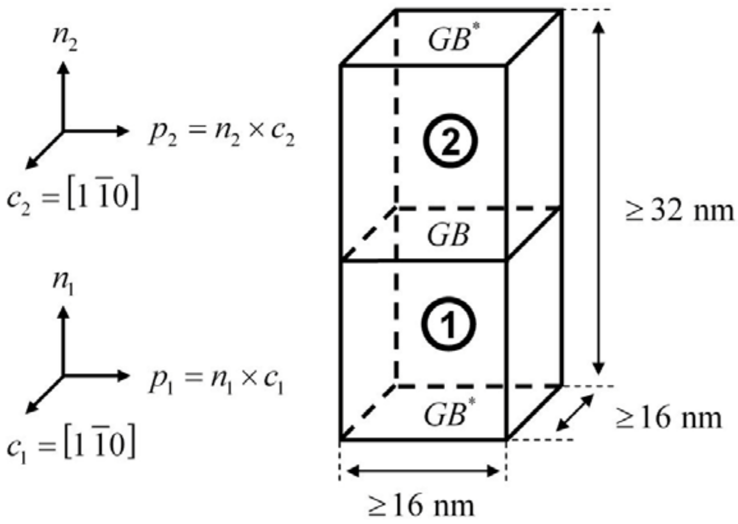
Simulation Methodology

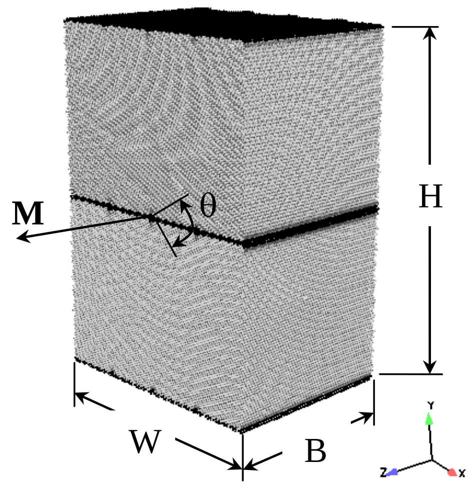
FCC EAM Potentials

- Copper (and Aluminum)
- Mishin and coworkers (1999, 2001) EAM potentials provide a relatively accurate description of unstable and stable stacking fault energy

Minimum Energy Grain Boundary Starting Configuration

- 3D periodic simulation cell
- Specify appropriate lattice directions
- Use a nonlinear conjugate gradient energy minimization w/ 2500+ starting configurations
- Expand dimensions to minimize sensitivity to simulation cell dimensions





Spearot, Tschopp, McDowell, Jacob, Acta Mat (2007) 705;
Tschopp, McDowell, IJP (2008) 191.

Simulation Methodology

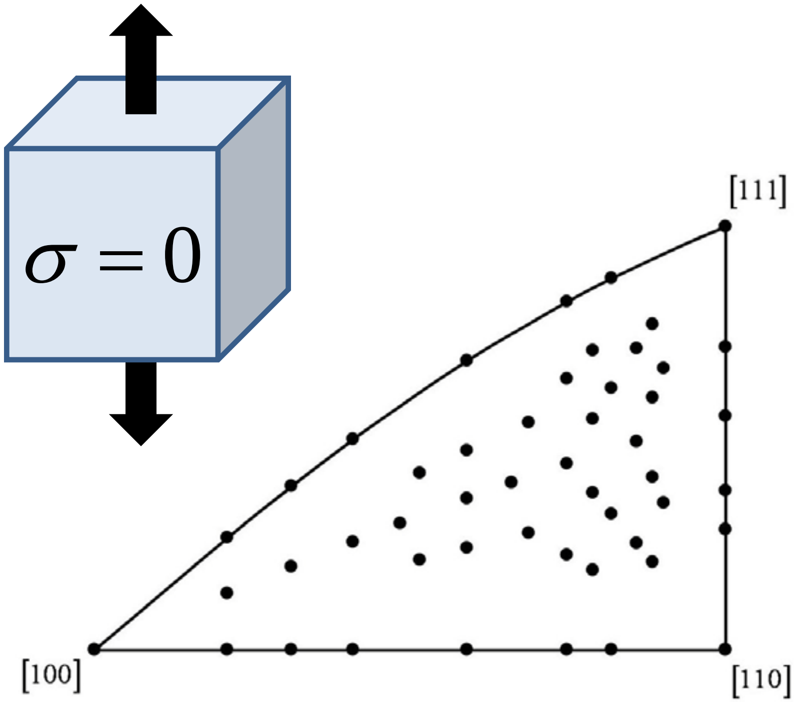
Single Crystal Configurations

- 49 loading axis orientations used for starting configurations with minimum edge dimension of 16 nm

Uniaxial Tensile/Compressive Deformation

- Equilibrate at temperature
- Uniaxial strain of 10^9 s^{-1} in the loading direction (*e.g.*, perpendicular to GB)
- Modified NPT equations of motion (Spearot et al. 2005) are used for the lateral boundaries
- Strain until dislocation nucleation

$$\dot{\varepsilon} = 10^9$$

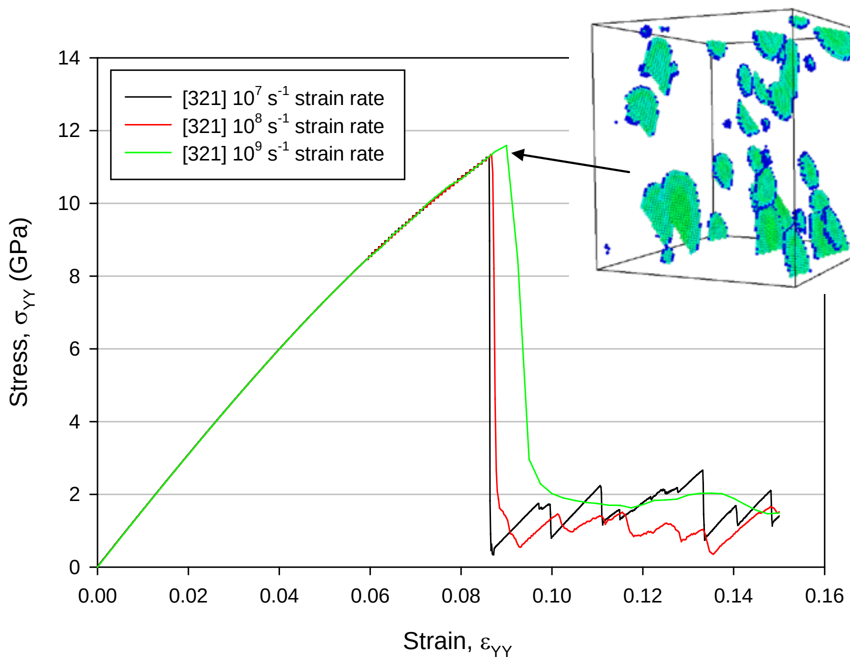


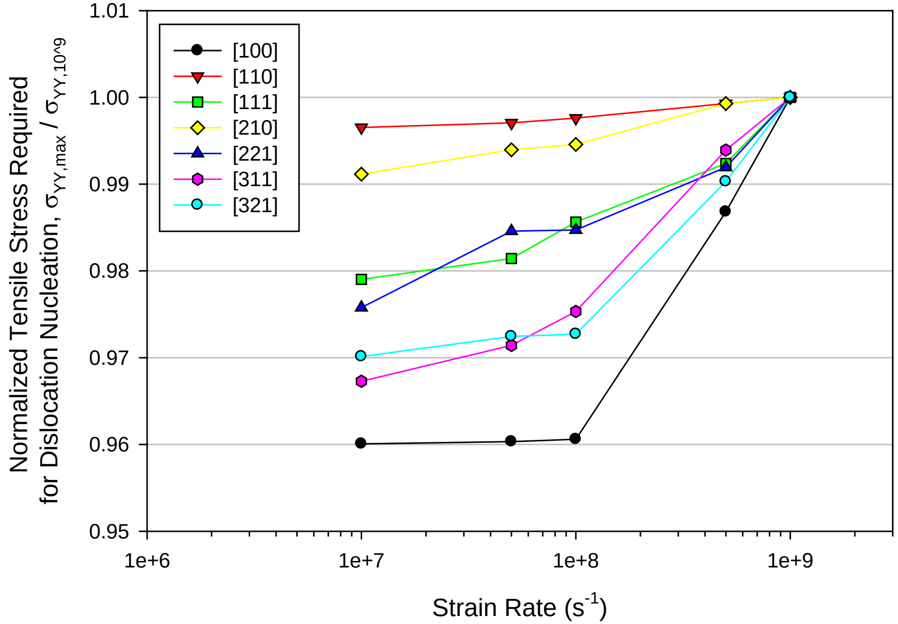
Stereographic triangle showing the 49 uniaxial loading axis orientations investigated in the single crystal deformation simulations.

Tschopp, Spearot, McDowell, MSMSE (2007) 693;
Tschopp, McDowell JMPS (2008);
Tschopp, McDowell APL (2007)

Strain Rate Dependence of Dislocation Nucleation Stress

"Orientation and Rate Dependence of Dislocation Nucleation Stress Computed using Molecular Dynamics"





As the strain rate is reduced from 10^9 to 10^7 s^{-1}, the tensile stress required for dislocation nucleation is reduced by at most 4%.

Spearot, Tschopp, McDowell, Scripta Materialia (2009)

Bicrystal Simulations

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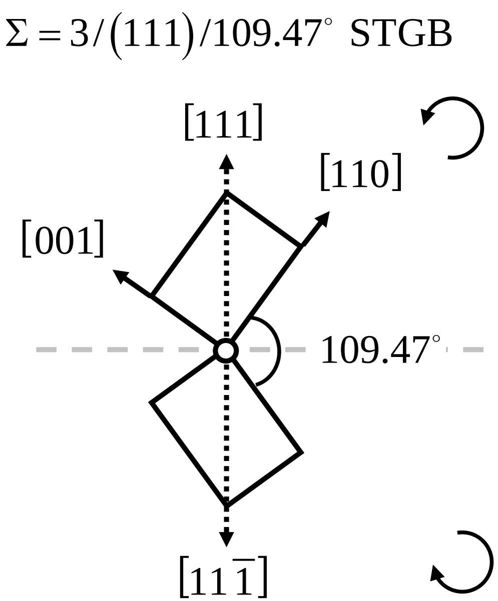
Grain Boundary Degrees of Freedom

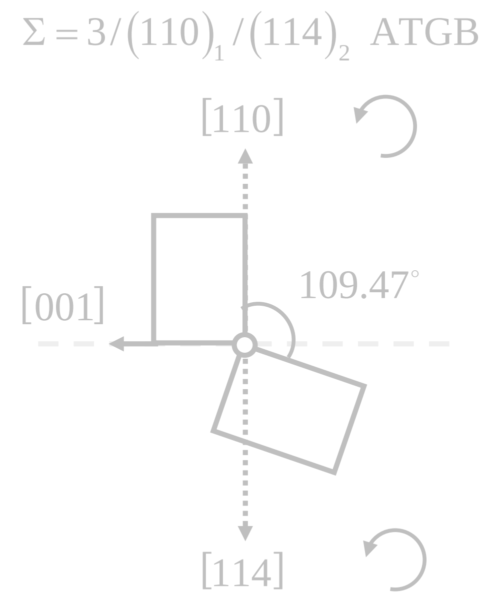
Asymmetric tilt grain boundaries are the most experimentally observed boundaries in polycrystals (Rohrer, Rollett, et al.).



(a)

STGB

- Rotated about tilt direction, <110> here
- Lattices **ARE** symmetric about GB plane
- Slip planes of MRSS **ARE** of the same geometric relationship with the GB plane, *i.e.*, Schmid factor ***is*** equal in both lattices



(b)

Symmetric (a) and *asymmetric* (b) tilt grain boundaries in the Σ3 system.

Tschopp, McDowell, Phil Mag (2007) 3147.

Grain Boundary Degrees of Freedom

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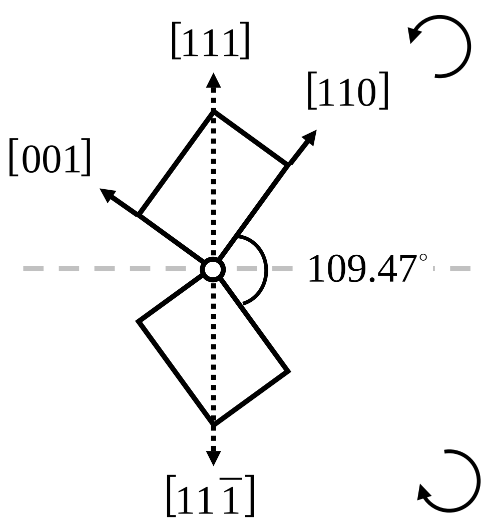
$\Sigma = 3/(111)/109.47^{\circ}$ STGB

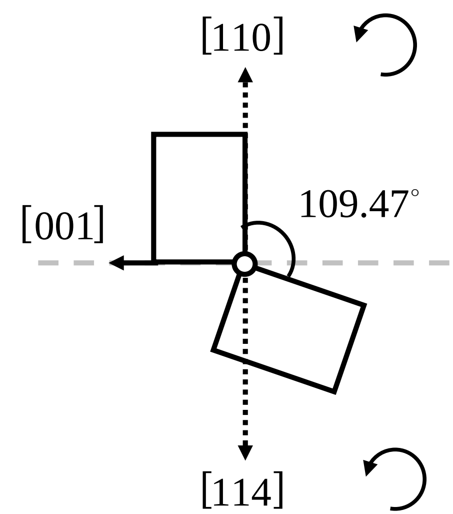


(a)

ATGB →

- Lattices **ARE NOT** symmetric about GB plane
- Slip planes of MRSS **ARE NOT** of the same geometric relationship with the GB plane, *i.e.*, Schmid factor ***is not*** equal in both lattices

$\Sigma = 3/(110)_1/(114)_2$ ATGB



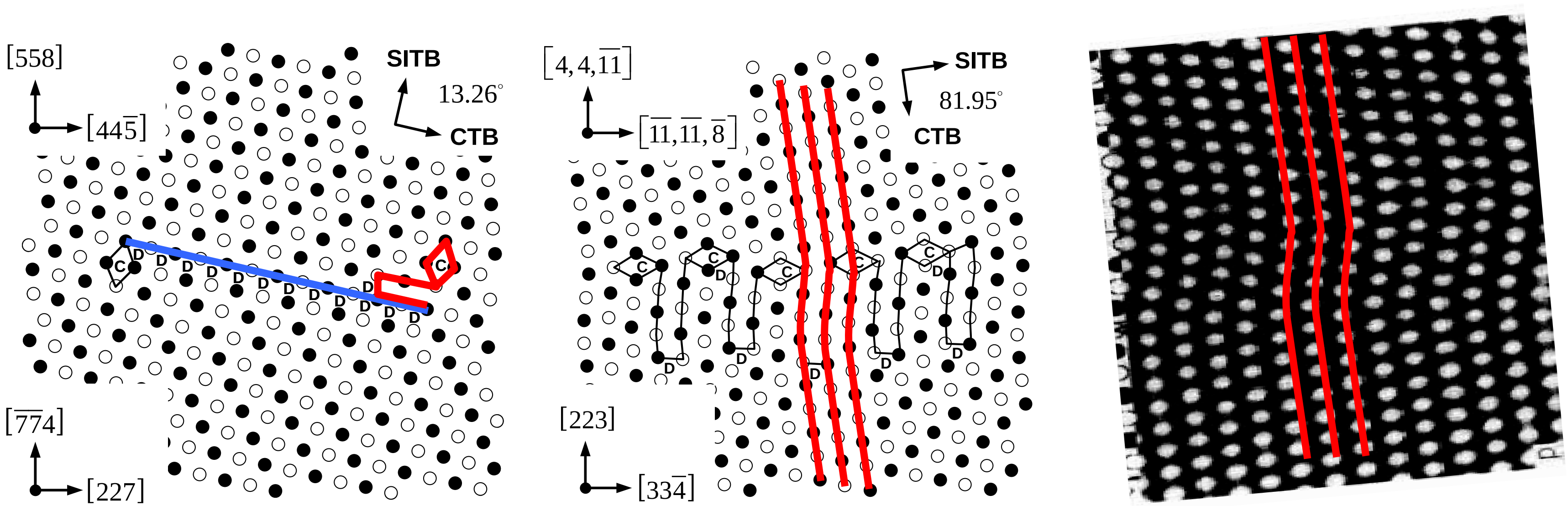
(b)

Symmetric (a) and *asymmetric* (b) tilt grain boundaries in the Σ3 system.

Tschopp, McDowell, Phil Mag (2007) 3147.

Grain Boundary Characterization

The structure, energy and free volume of symmetric and asymmetric tilt grain boundaries can provide insight into interfacial properties, such as dislocation nucleation.



Grain boundary structures of a few Σ3 asymmetric boundaries in Cu compared to HRTEM images in Ag (Ernst *et al*. 1992).

Tschopp, McDowell, Phil Mag, 87 (2007) 3147;
Tschopp, McDowell, J. Materials Science (2007)

Grain Boundary Characterization

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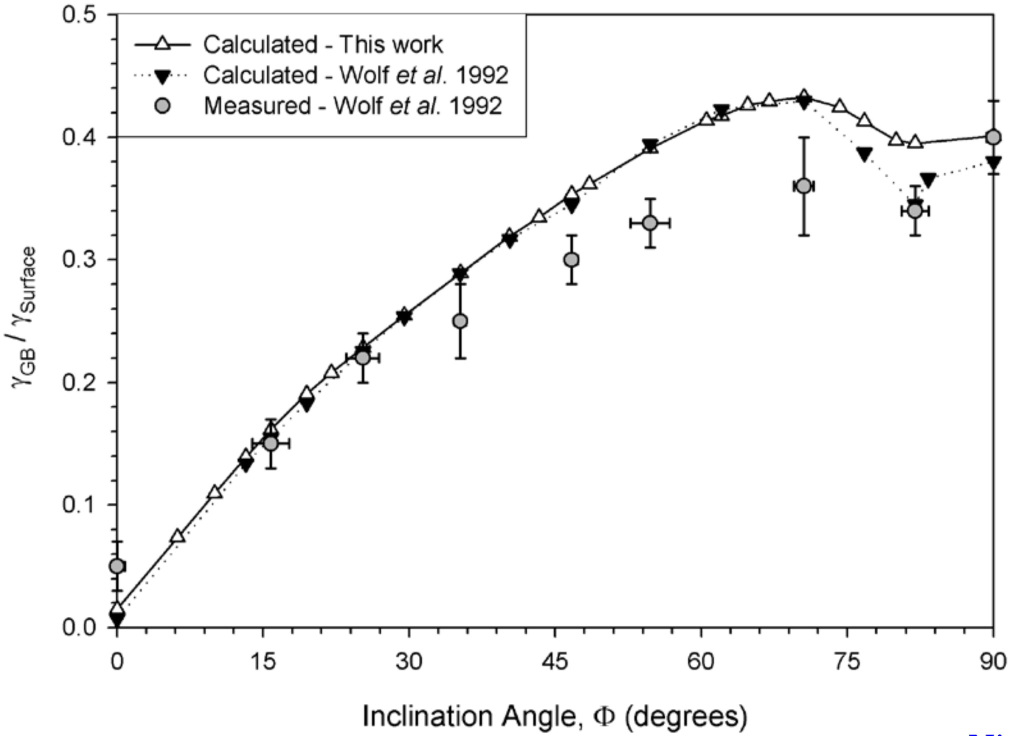


CSL ATGB systems investigated:

Σ3, Σ5, Σ9, Σ11, Σ13

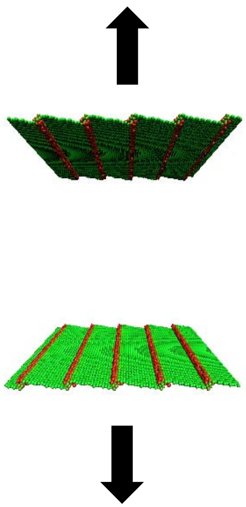
** Most extensive atomistic work on ATGB energy and structure in Cu & Al*

Tschopp and McDowell, Phil Mag, 87 (2007) 3147;
Tschopp and McDowell, Phil Mag, 87 (2007) 3871.

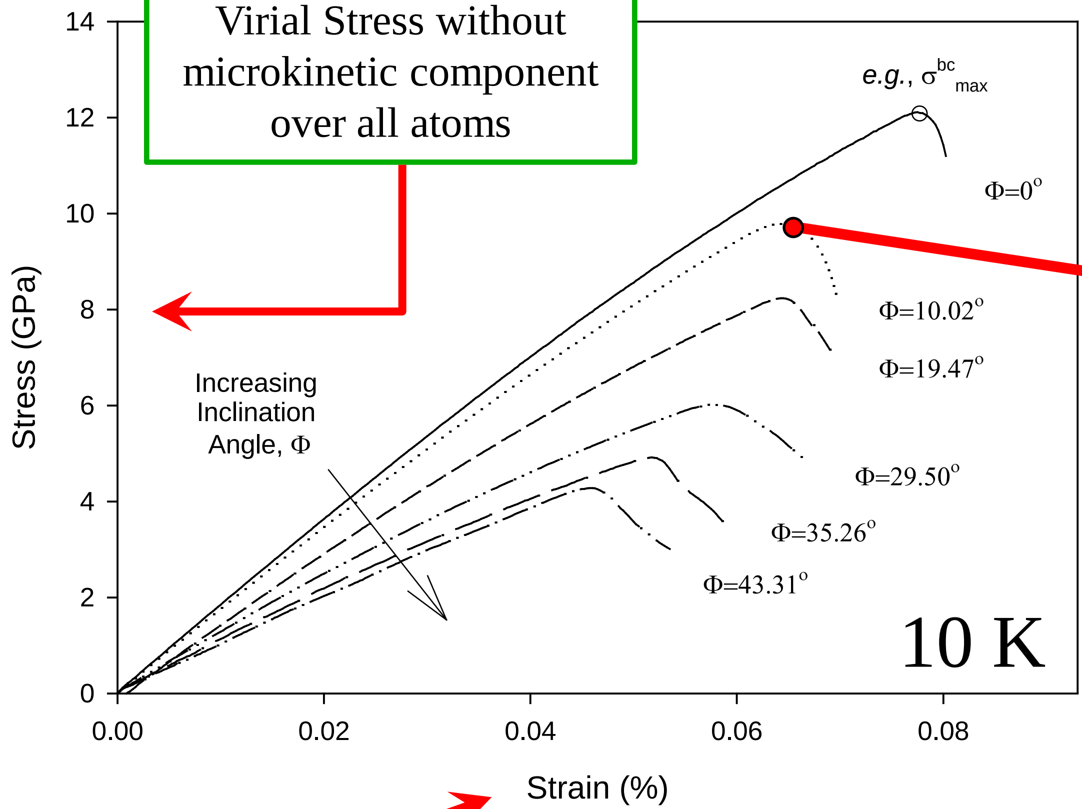
Ni/Al grain boundaries, see Olmsted, Foiles, Holm, Acta Materialia (2009).

Grain Boundary Dislocation Nucleation

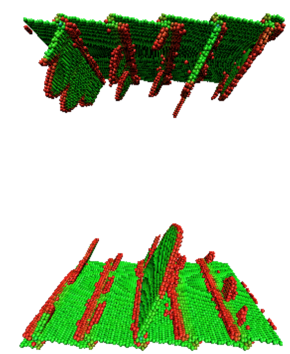
Uniaxial Tension



Virial Stress without microkinetic component over all atoms



$\Sigma 3$ ATGBs

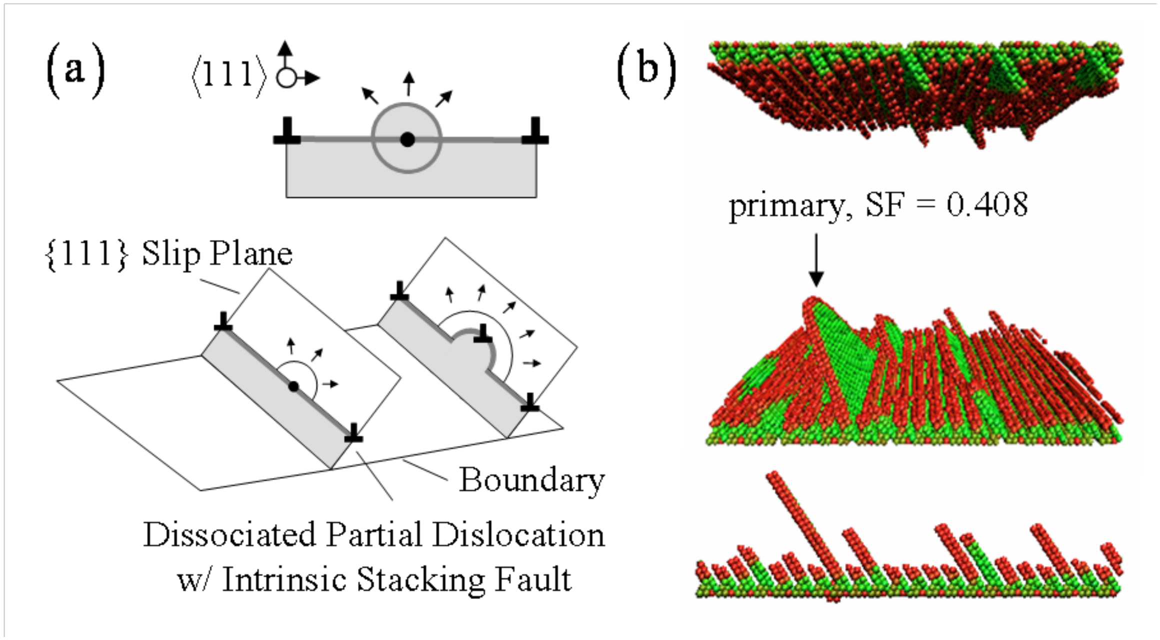


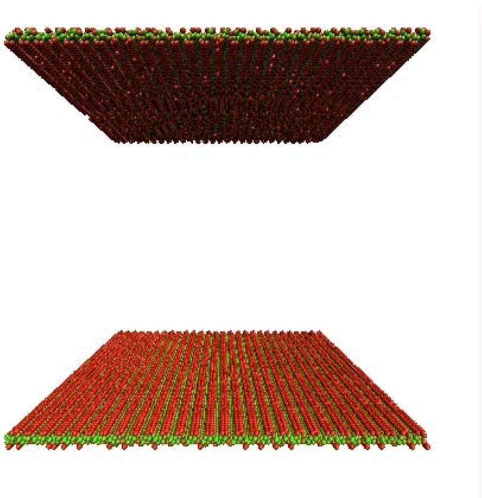
Strain measured over entire length of simulation cell

The maximum tensile stress corresponds to dislocation nucleation and emission from the $\Sigma 3$ asymmetric tilt GBs.

Spearot, Tschopp, McDowell, Jacob, Acta Mat (2007) 705;
Tschopp, McDowell, IJP (2008) 191.

Grain Boundary Dislocation Nucleation Mechanisms





Dislocations initially dissociate from the boundary and then are emitted into the lattice.

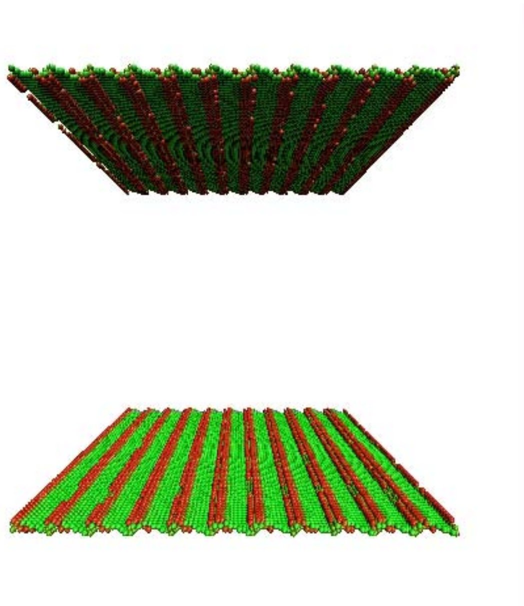
LOW Dislocation Nucleation Stress

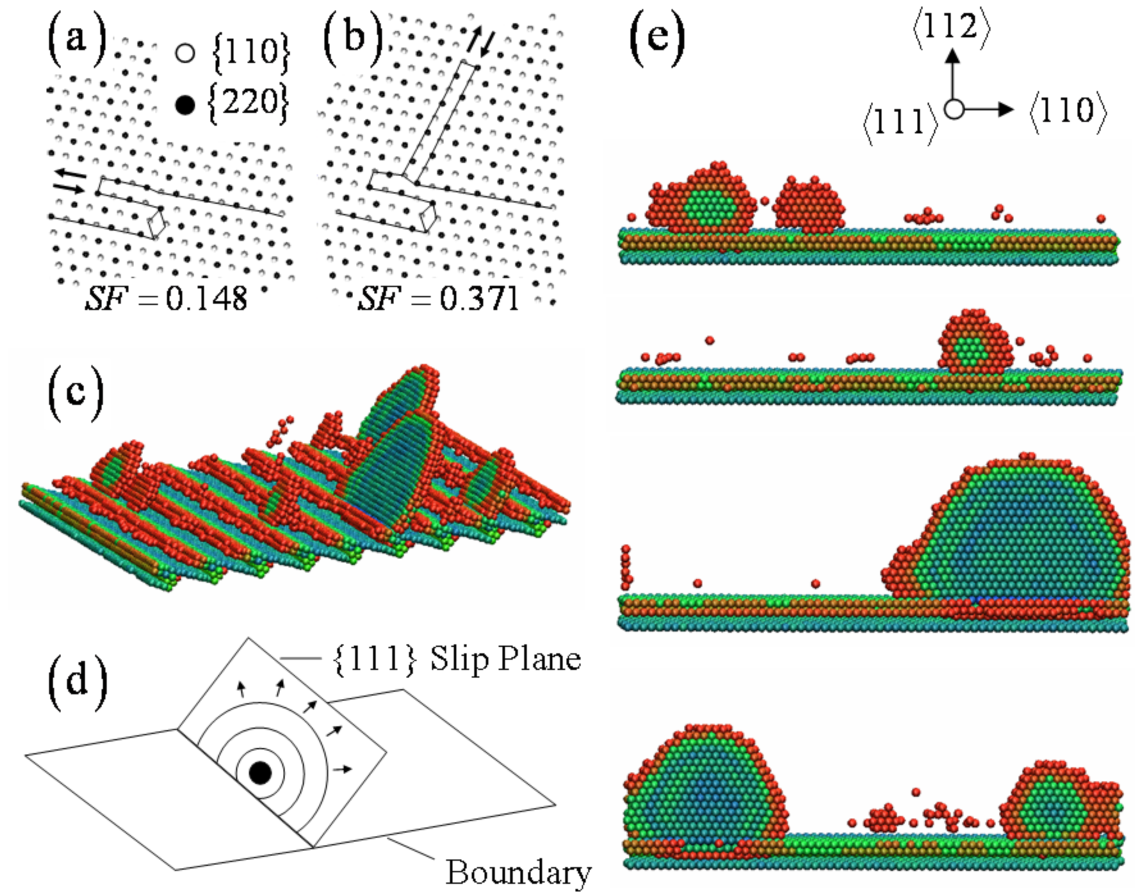
Highlighted recently in, Derlet, Gumbsch, Hoagland, J. Li, McDowell, Van Swygenhoven, and J. Wang, March 2009 MRS Bulletin

Tschopp, McDowell, Scripta Materialia 58 (2008) 299.

Grain Boundary Dislocation Nucleation Mechanisms

Dislocation loops nucleate homogeneously in the lattice.





HIGH Dislocation Nucleation Stress

Tschopp, McDowell, Scripta Materialia 58 (2008) 299.

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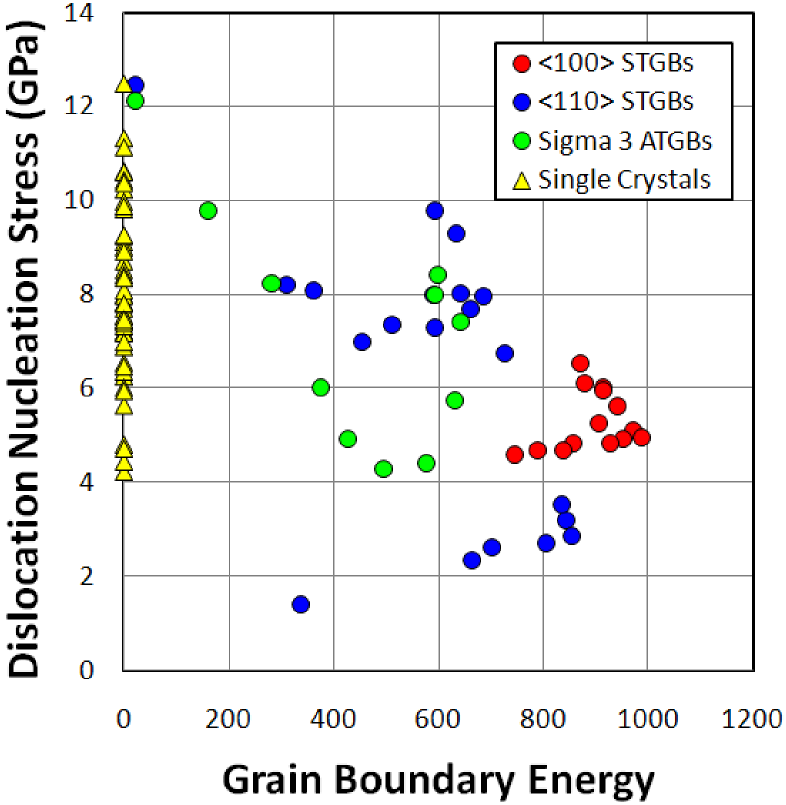
Dislocation Nucleation Stress

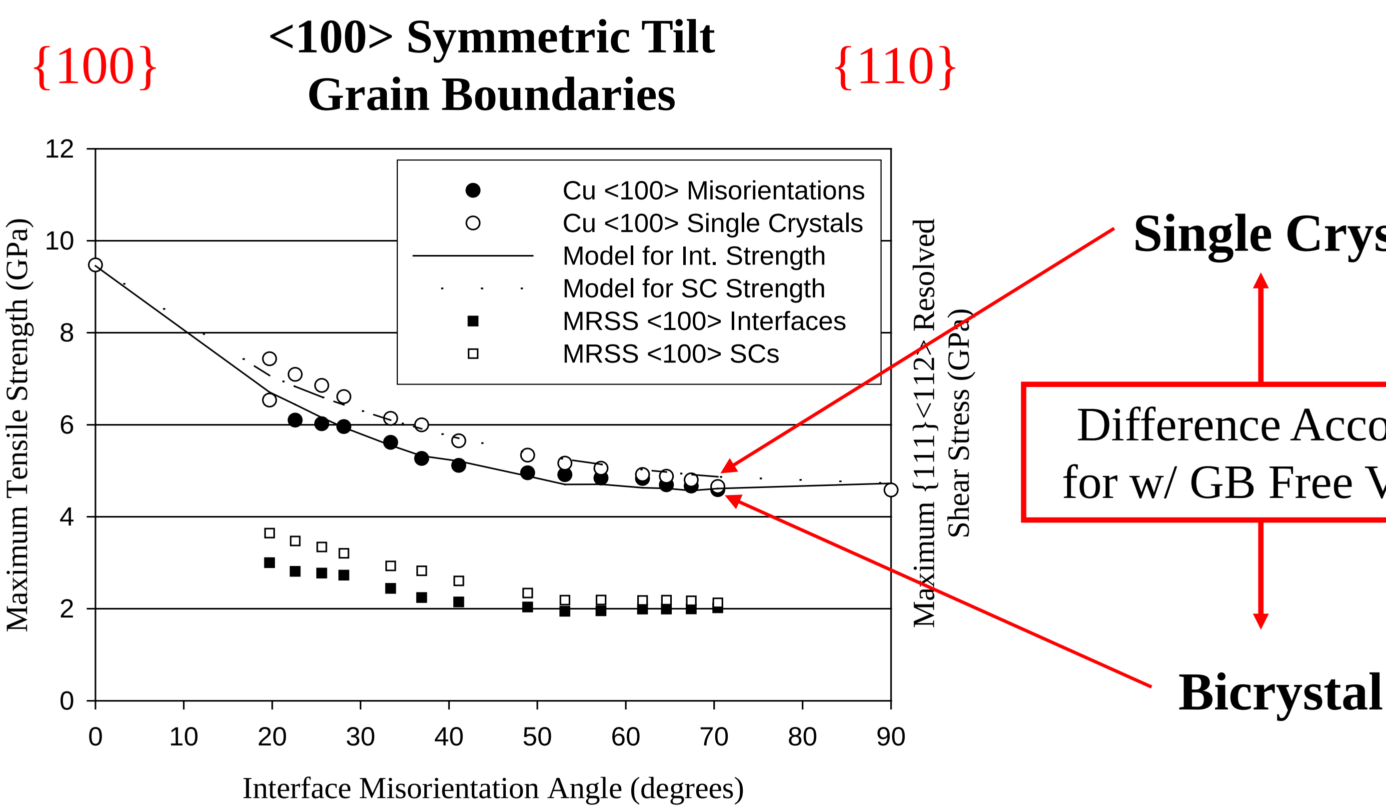


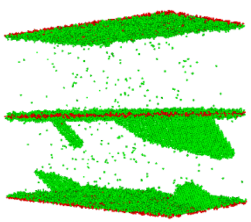
No apparent correlation with…

- **GB ENERGY**
- **MISORIENTATION ANGLE**
- **SIGMA VALUE**
- **FREE VOLUME**

Can we predict the dislocation nucleation stress using grain boundary metrics, e.g., the **grain boundary energy or** the **grain boundary misorientation angle**?

Dislocation Nucleation Stress



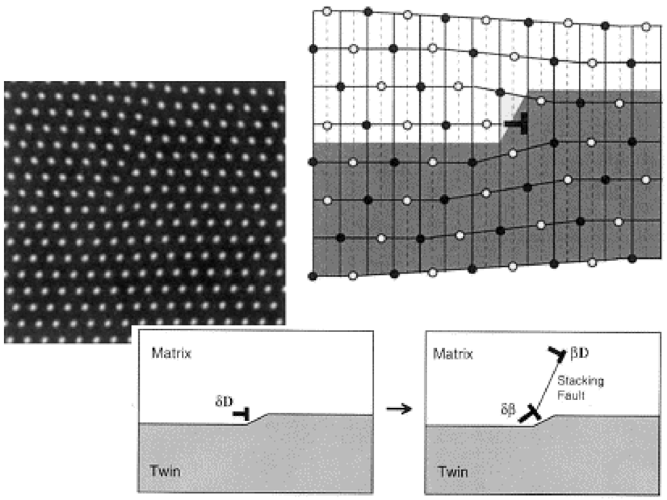


Can we predict the grain boundary dislocation nucleation stress from single crystal dislocation nucleation stresses?

(Later, this will be calculated from resolved stress components)

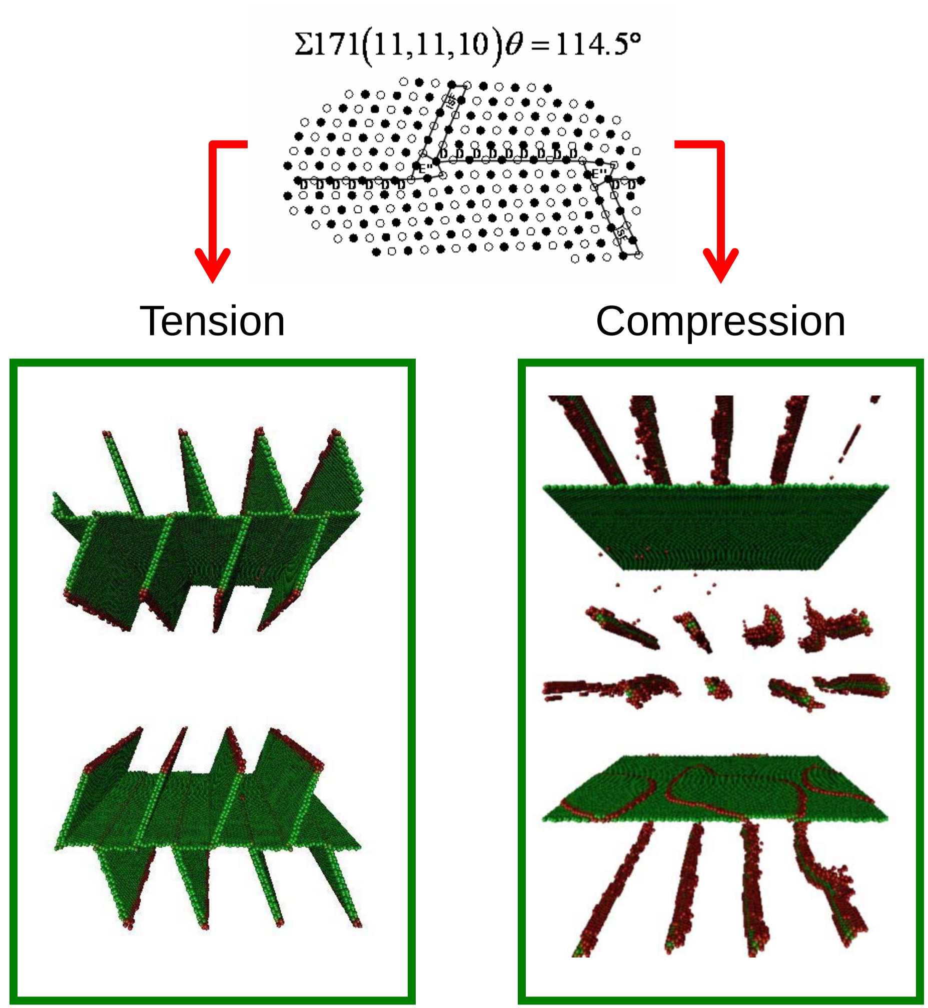
Spearot, Tschopp, Jacob, McDowell, Acta Materialia, (2007)

Tension-Compression Asymmetry



<u>1/3<111> Disconnection</u>

- Medlin, Carter, Angelo, Mills (1997)
- Medlin (1999, *Advances in Twinning*)
- Foiles and Medlin (2001)
- Marquis and Medlin (2005)
- Marquis, Medlin and Léonard (2007)



Σ171 Vicinal Twin
<110> Symmetric Tilt Boundary

Tschopp, Tucker, McDowell, Acta Mat (2007) 3959;
Tschopp, Tucker, McDowell, Comp Mat Sci (2008).

Heterogeneous dislocation nucleation findings

- Grain boundary structure plays an important role in dislocation nucleation mechanism

- **Heterogeneous** nucleation stress in grain boundaries is related to the **homogeneous** nucleation stress of the crystal lattice
  - Nucleation stress ***IS NOT*** correlated with energy, Σ content, disorientation angle, or excess free volume
  - **(LATER)** Single crystal nucleation stress ***IS*** related to resolved stresses (Schmid stress, normal stress)

- Tension-compression asymmetry in dislocation nucleation
  - Partial dislocations nucleate in tension, full dislocations in compression
    - **(LATER)** Normal stress! Shear stress in opposite directions.

Single Crystal Simulations

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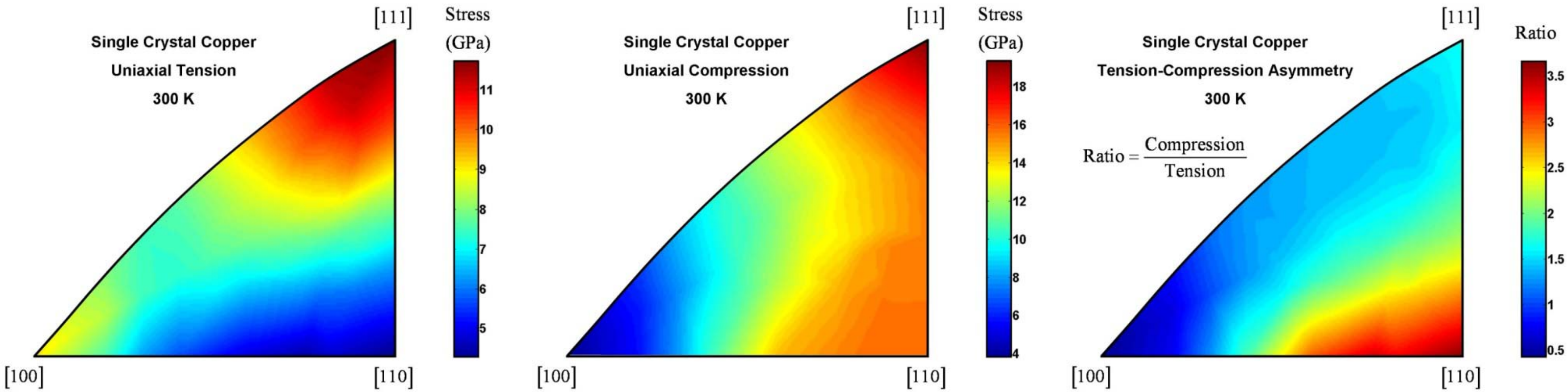
Orientation Dependence of Dislocation Nucleation Stress

Tension | Compression | Tension-Compression



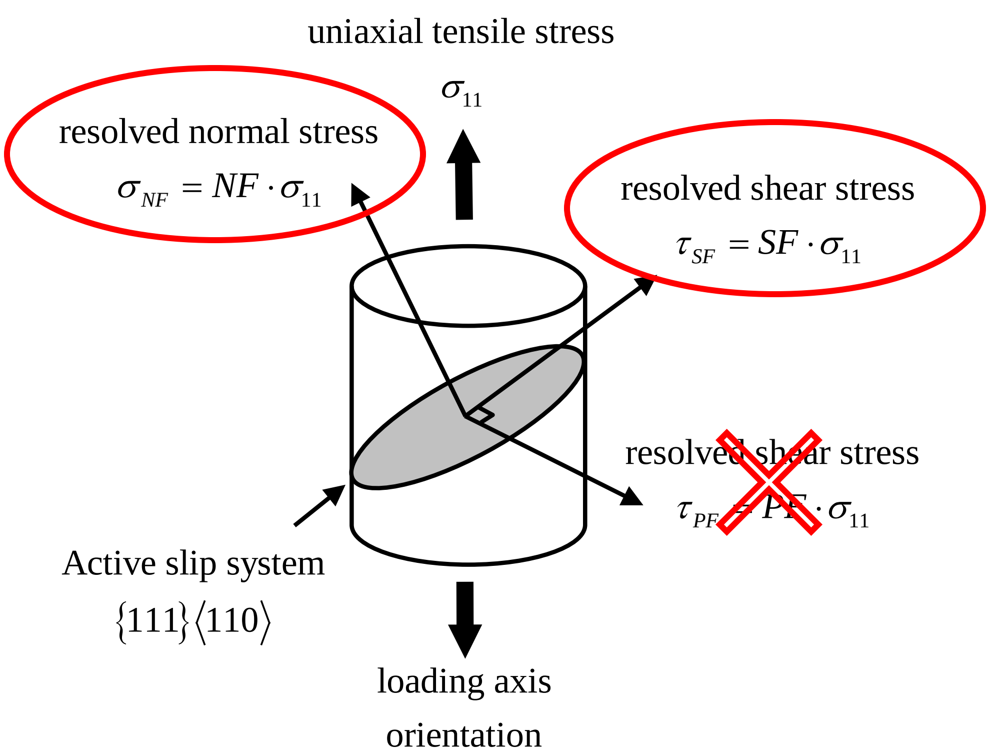
<u>~ 200 simulations in tension and compression</u>

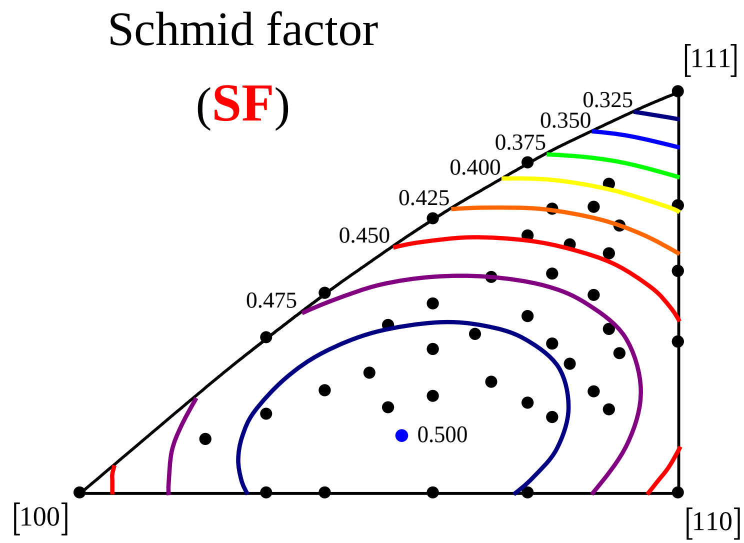
• Dislocation nucleation is highly orientation-dependent, with different dependences in tension and compression.

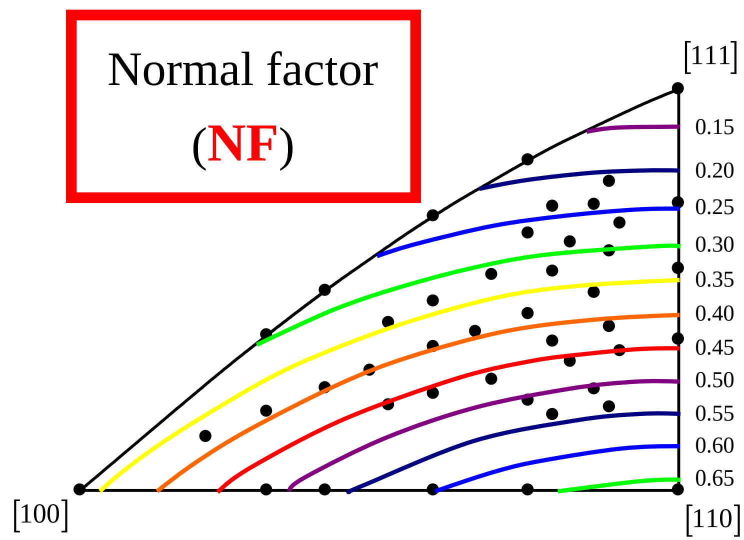
• Dislocation nucleation stresses <u>should</u> be related to the resolved stress components in FCC Copper, i.e., the Schmid resolved shear stress?

Tschopp, McDowell, APL 90 (2007) 121916

Resolved Stress Components





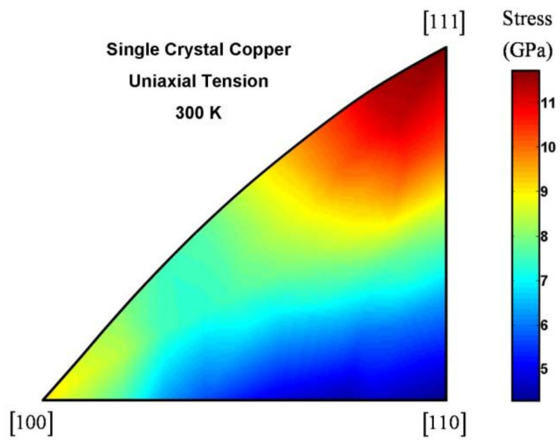


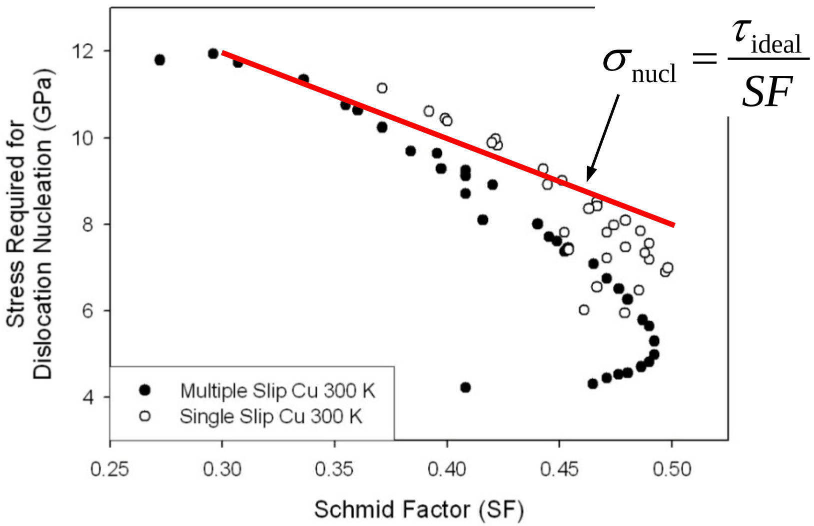
Dislocation nucleation tends to follow both the Schmid resolved shear stress and the non-Schmid resolved normal stress.

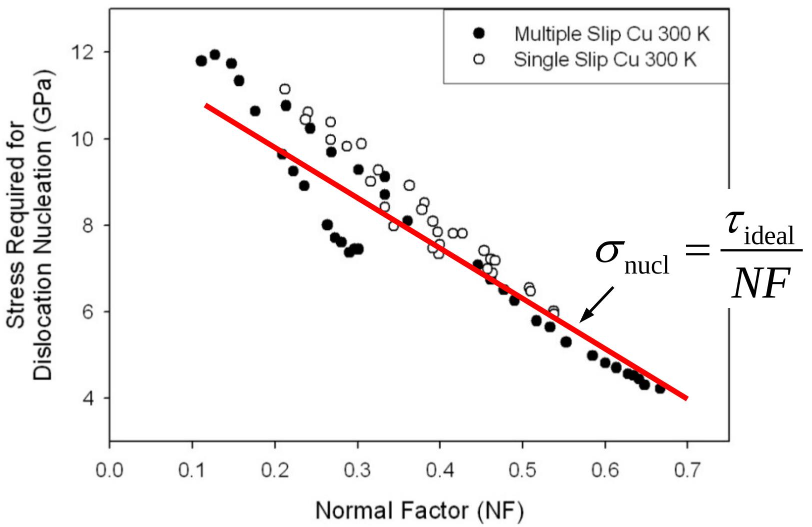
Spearot, Tschopp, Jacob, McDowell, Acta Materialia (2007) 705;
Tschopp, Spearot, McDowell, MSMSE (2007) 693

Resolved stress components and the dislocation nucleation stress

Tension







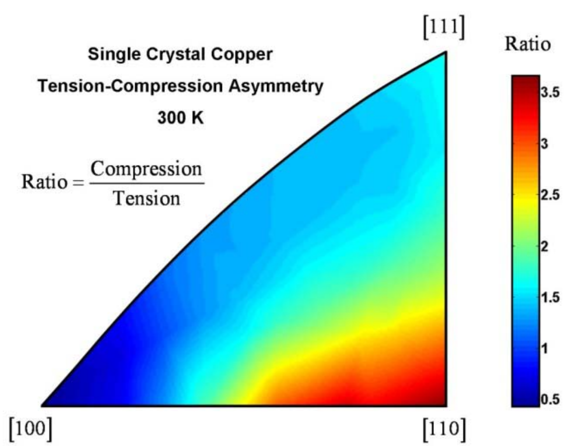
For dislocation nucleation in tension, the following trends emerge:

- the **higher** the Schmid factor, the **lower** the dislocation nucleation stress
- the **higher** the "normal" factor, the **lower** the dislocation nucleation stress

Tschopp, McDowell, JMPS (2008) 1806

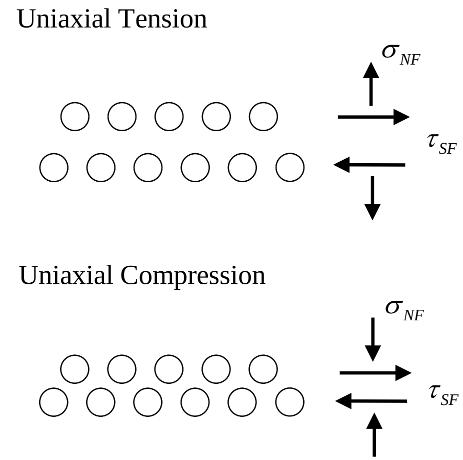
Resolved stresses and tension-compression asymmetry in dislocation nucleation stress

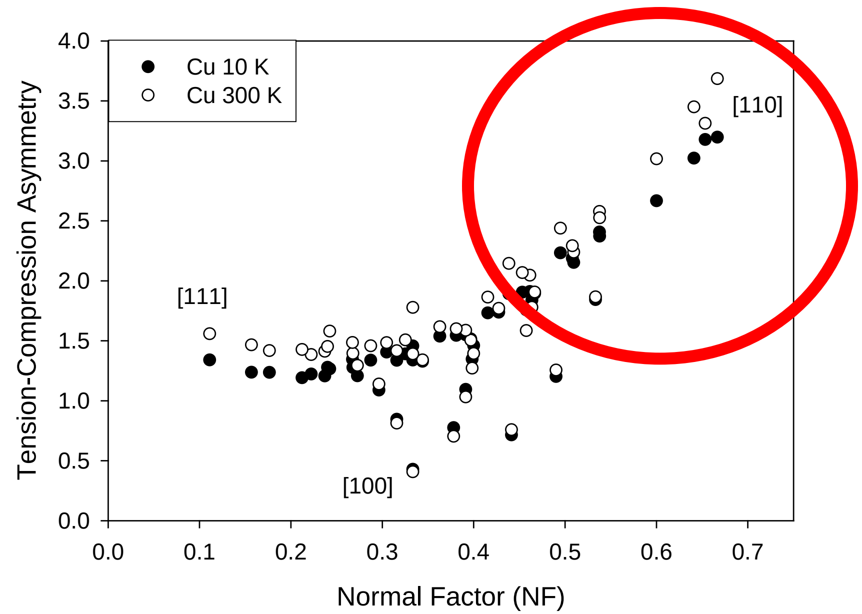
Tension-Compression



For dislocation nucleation, the following trends emerge:

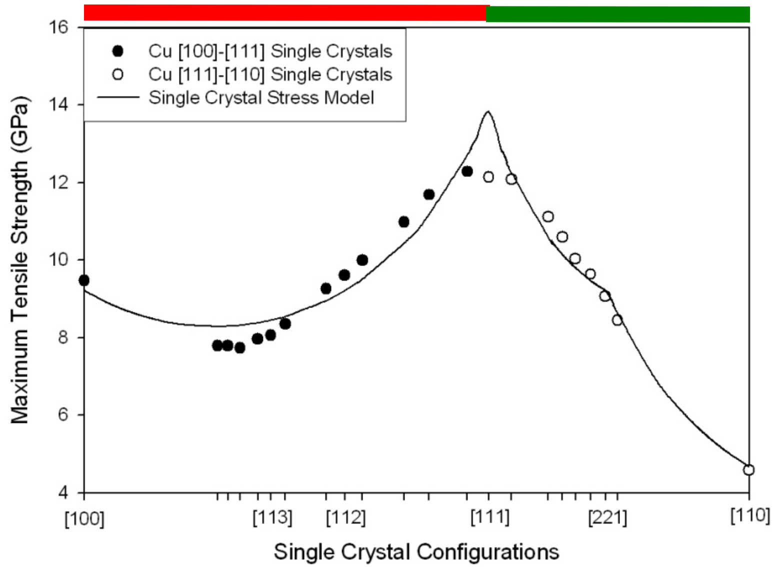
• **High** "normal" factor orientations have a **higher** tension-compression asymmetry in dislocation nucleation stress

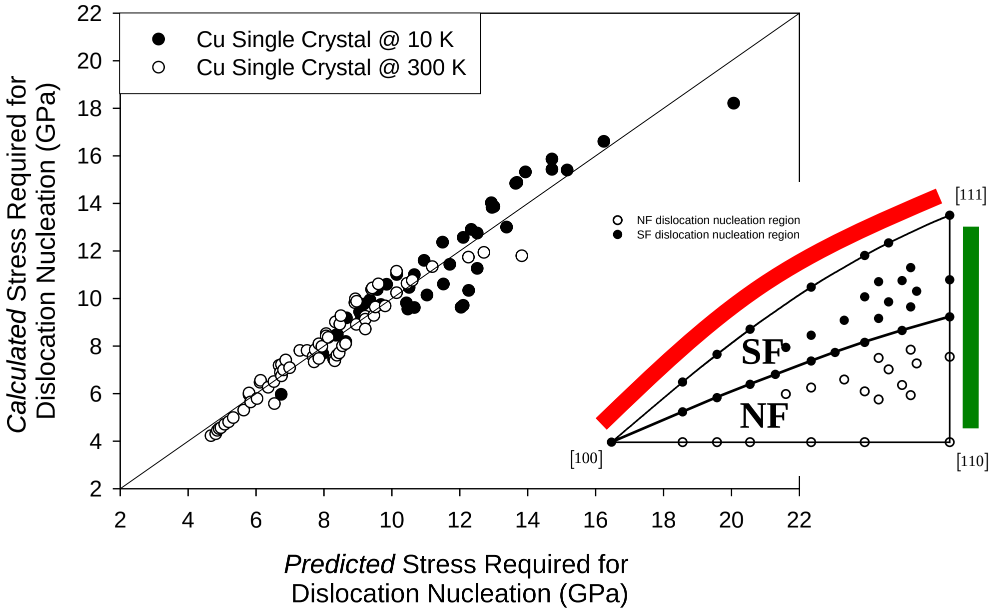




Tschopp, McDowell, APL 90 (2007) 121916;
Tschopp, McDowell, JMPS (2008) 1806

Dislocation nucleation stress model





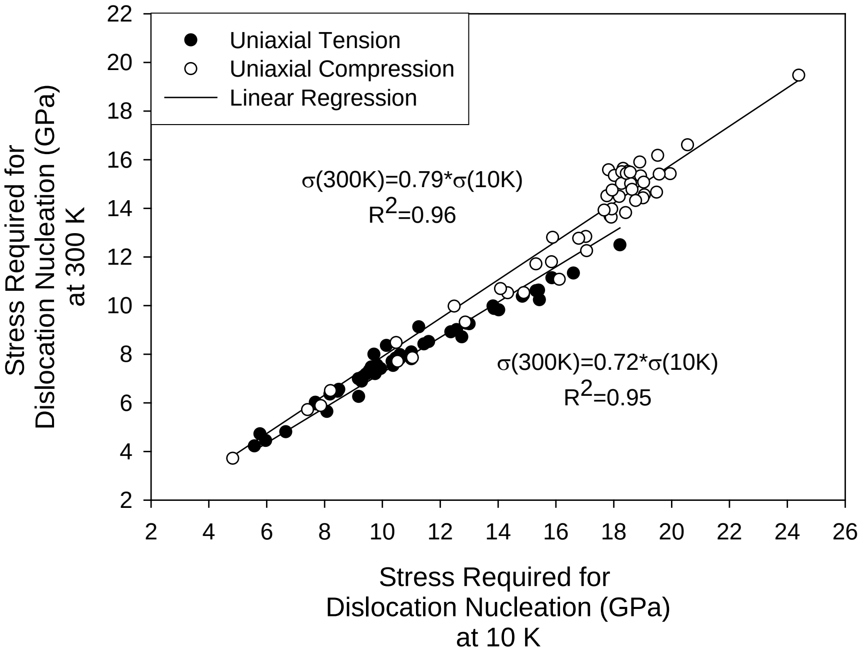
Classical Schmid Law $$\sigma_{\text{motion}} = \frac{\tau_{\text{ideal}}}{SF}$$

w/ non-Schmid normal stress component $$\sigma_{\text{nucl}} = \frac{\tau_{\text{ideal}}}{\alpha_{\text{SF}} SF + \alpha_{\text{NF}} NF}$$

In single crystal FCC Cu, the **non-Schmid normal stress** plays an important role in the dislocation nucleation stress.

Spearot, Tschopp, McDowell, Acta Materialia (2007) 705;
Tschopp, Spearot, McDowell, MSMSE (2007) 693

Activation energy, activation volume



Motivated by Zhu, Li et al. (2008)

$$\sigma_{\text{nucl}}(T=0K)=\frac{\tau_{\text{ideal}}}{\alpha_{\text{s}}SF+\alpha_{\text{n}}NF}=\frac{Q^*}{\Omega}$$

$$\sigma_{\text{nucl}}(T)=f(T)\left[\sigma_{\text{nucl}}(T=0K)\right]$$

$$f(T)=1-\frac{k_BT}{Q^*}\ln\frac{k_BTN\nu_0}{\Omega E\dot{\varepsilon}}$$

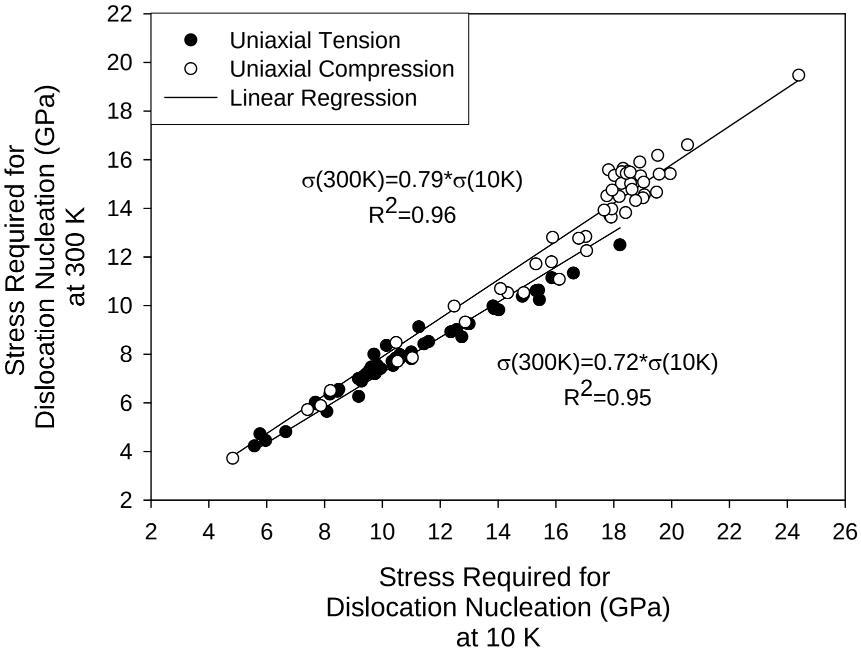
Ω Activation volume

Q^* Activation energy $(\sigma=0)$

Q Activation energy

Tschopp, McDowell, JMPS (2008) 1806

Activation energy, activation volume



Motivated by Zhu, Li et al. (2008)

$$\sigma_{\text{nucl}}(T=0K)=\frac{\tau_{\text{ideal}}}{\alpha_{\text{s}}SF+\alpha_{\text{n}}NF}=\frac{Q^*}{\Omega}$$

$$\sigma_{\text{nucl}}(T)=f(T)\left[\sigma_{\text{nucl}}(T=0K)\right]$$

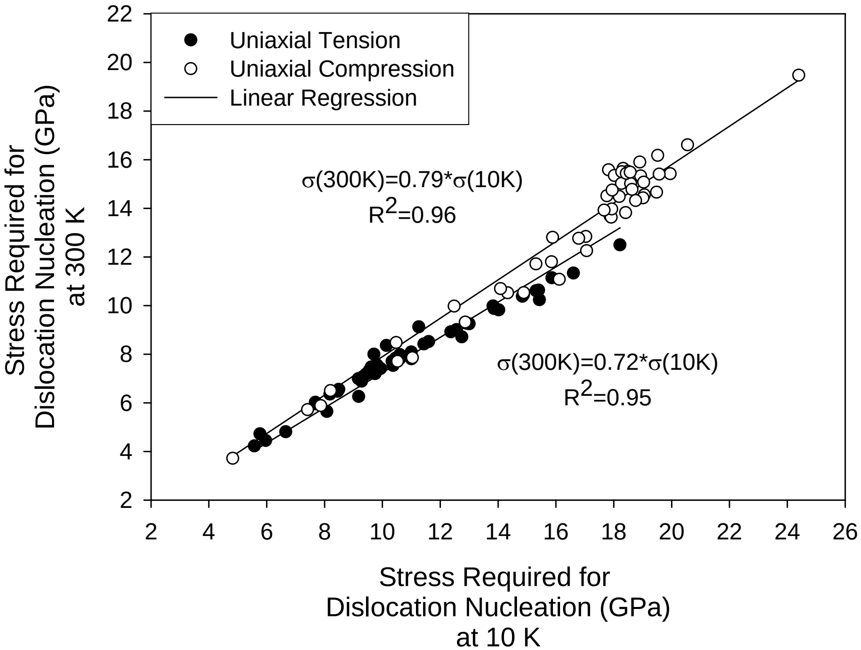
$$f(T)=1-\frac{k_BT}{Q^*}\ln\frac{k_BTN\nu_0}{\Omega E\dot{\varepsilon}}$$

Ω	Activation volume	$\approx$ 0.6-2.2 b^3
Q^*	Activation energy ($\sigma=0$)	$\approx$1.1-1.9 eV
Q	Activation energy	$\approx$ 0.3 eV

Homogeneous dislocation nucleation has activation volumes & energies on the order of heterogeneous dislocation nucleation

Tschopp, McDowell, JMPS (2008) 1806

Activation energy, activation volume



Schuh, Mason, et al., (2005)
Nanoindentation on Pt

$\Omega_{expt} \approx 0.5\,b^3$

Q_{expt} 0.28 eV

T. Zhu, J. Li, et al., (2007, 2008)
CINEB on nanopillars & boundaries

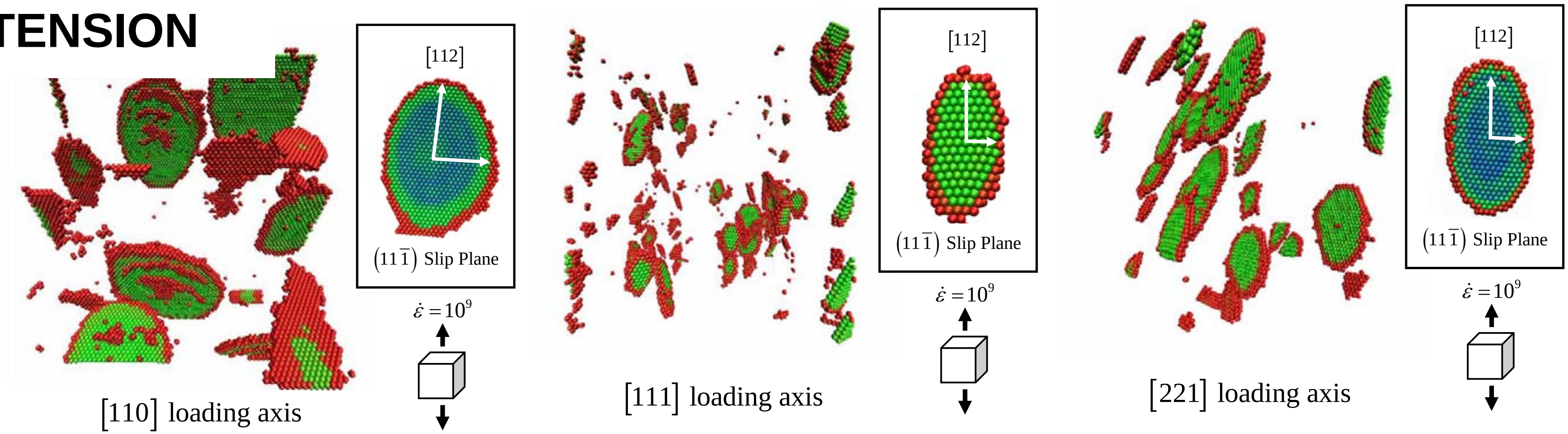
$Q_{side\ surface}$	0.64 eV
Q_{corner}	0.1 eV
$Q_{disl\ absorption}$	0.49 eV
$Q_{disl\ transmission}$	0.67 eV

Ω	Activation volume	$\approx$ 0.6-2.2 b^3
Q^*	Activation energy ($\sigma = 0$)	$\approx$ 1.1-1.9 eV
Q	Activation energy	$\approx$ 0.3 eV

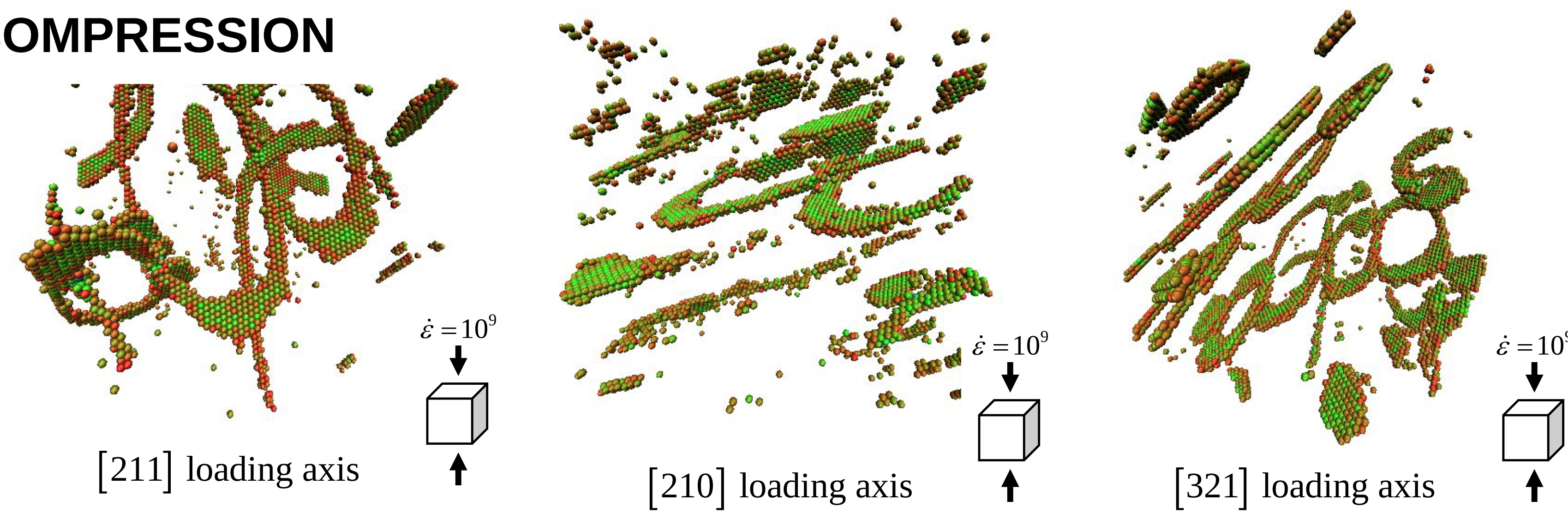
Tschopp, McDowell, JMPS (2008) 1806

Dislocation mechanisms

TENSION

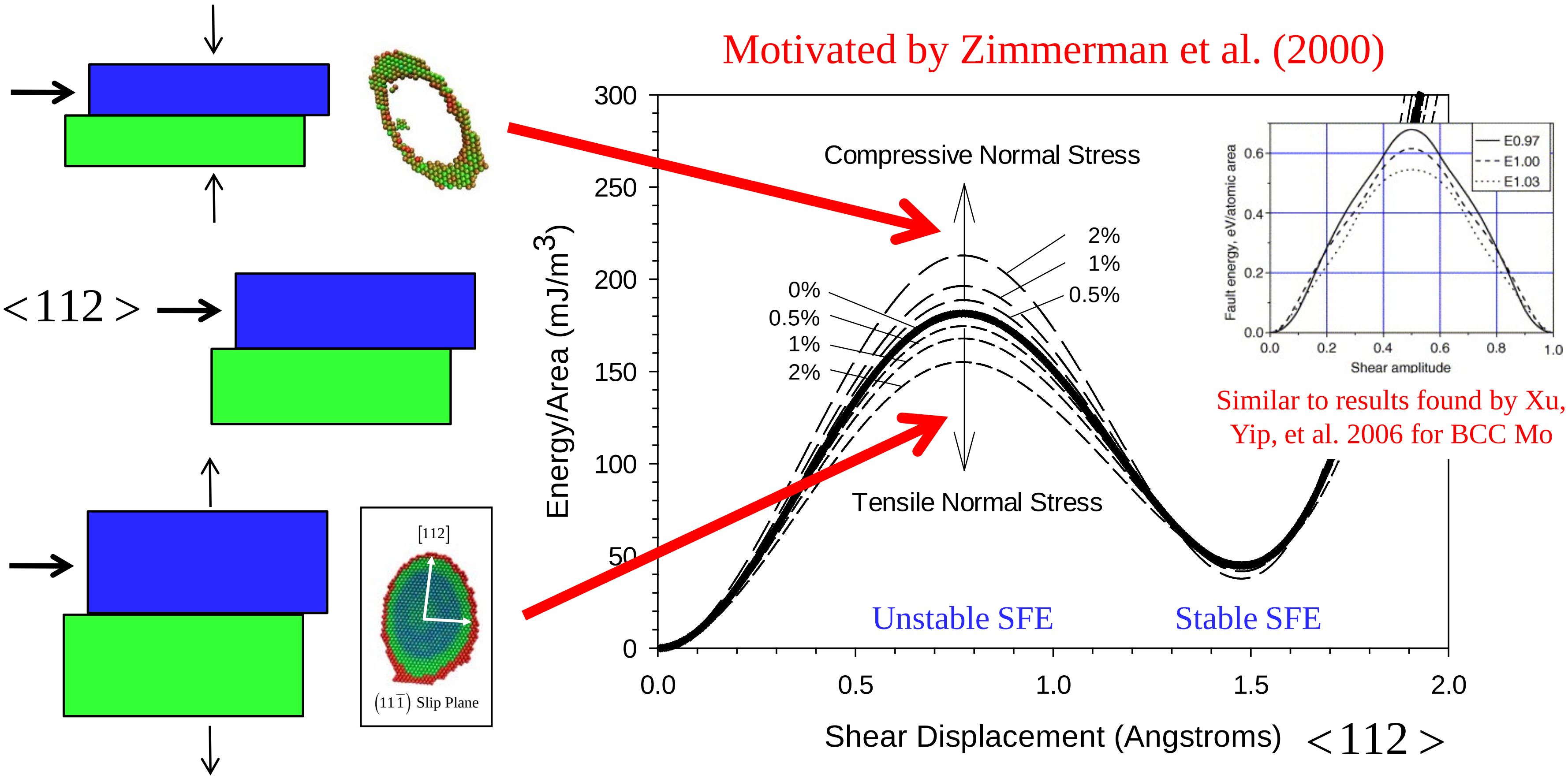


COMPRESSION



Tschopp, McDowell, JMPS (2008) 1806

Generalized Stacking Fault Energy Curve



The ratio of stable to unstable stacking fault energy, γ_{sf}/γ_{usf}, has been used to describe the partial/full dislocation behavior between FCC metals, where γ_{sf}/γ_{usf} of approximately 1 (i.e., Al) exhibits full dislocation loops (Van Swygenhoven et al., 2004).

Tension-Compression behavior shown here does not follow this trend for Cu.

Homogeneous dislocation nucleation findings

- Resolved normal stress plays an important role in **homogeneous** *dislocation nucleation* (unlike *dislocation motion*)
  - *Also important for explaining tension-compression asymmetry in dislocation nucleation*

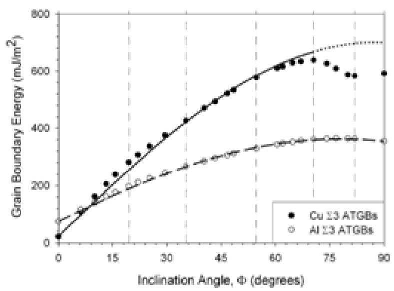
- *Activation energies* (~0.30 eV) and *activation volumes* (~1 b^3) are on the order of those calculated for heterogeneous dislocation nucleation

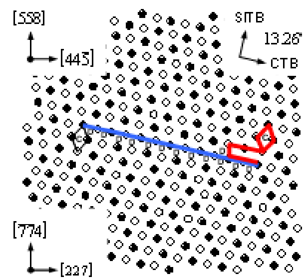
- Mechanisms - Partial dislocations nucleate in tension, full dislocations in compression
  - Unstable stacking fault energy on GSF curve
  - Influence of normal stress

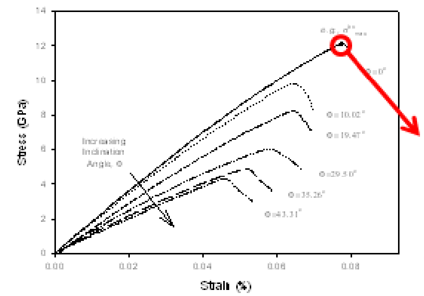
Conclusion

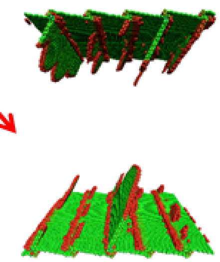
Energy ⟷ Boundary Structure ⟷ Dislocation Nucleation

Bicrystal Simulations of Dislocation Nucleation





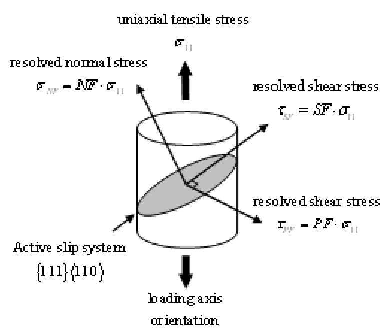


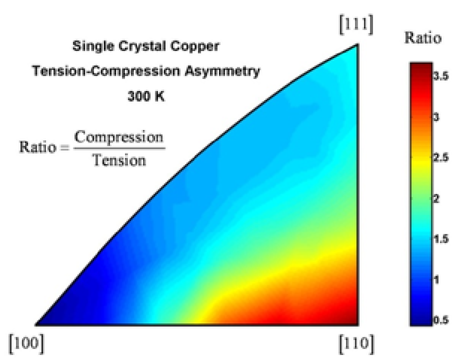


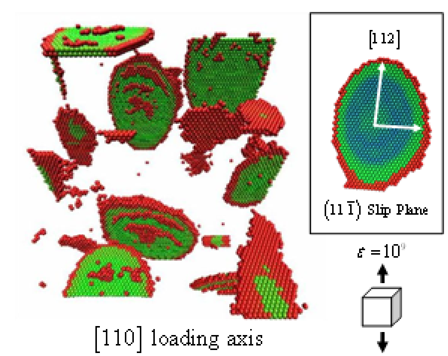
NORMAL STRESS

Resolved Stress ⟷ Lattice Stress Effect ⟷ Dislocation Nucleation

Single Crystal Simulations of Dislocation Nucleation







Thank you!

Questions?

Dissertation (free online):

Tschopp, M.A., “Atomistic simulations of dislocation nucleation in single crystals and grain boundaries”

http://smartech.library.gatech.edu/dspace/bitstream/1853/16239/1/tschopp_mark_a_200708_phd.pdf

GOOGLE: “tschopp” and “ETD”