Strengthening Trends of Nanovoid Irradiation Defects with Meso-Scale PFDD Modelling

Ashley Roach[1*], Shuozhi Xu[2], D.J. Luscher[3], Daniel Gianola[1], Irene Beyerlein[1,4]

[1]Materials Department, UC Santa Barbara

[2]School of Aerospace and Mechanical Engineering, University of Oklahoma

[3]Theoretical Division, Los Alamos National Lab (LANL)

[4]Department of Mechanical Engineering, UC Santa Barbara

Outline

- Irradiated Materials
- Nanovoid Strengthening Literature
- Simulation Approach with PFDD
- Nanovoid Strengthening Trends
- Dominant Mechanisms

Motivation: Irradiated Materials

Irradiated Materials

Nanovoid Strengthening Literature

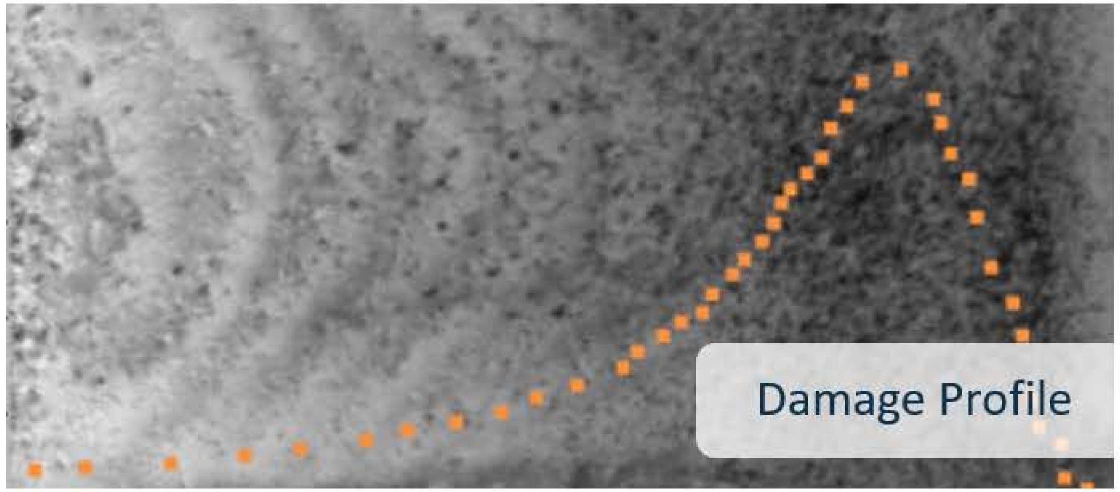
Simulation Approach with PFDD

Nanovoid Strengthening Trends

Dominant Mechanisms

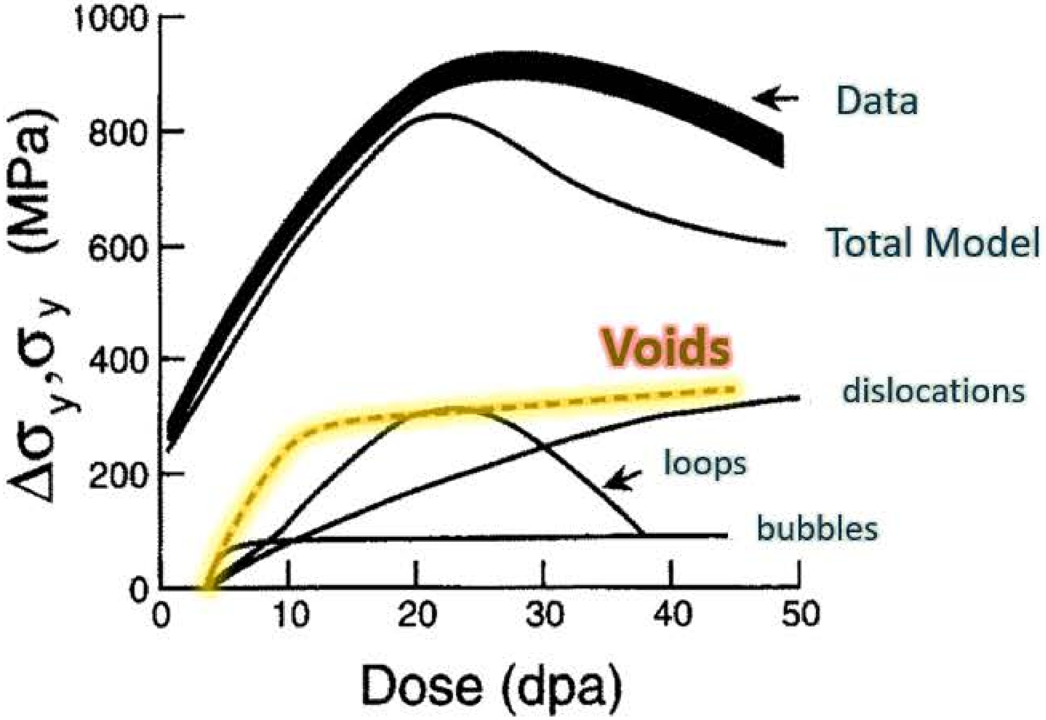
Nanovoids Contribute to Irradiation Strengthening

Irradiation Results in Very High Localized Defect Density

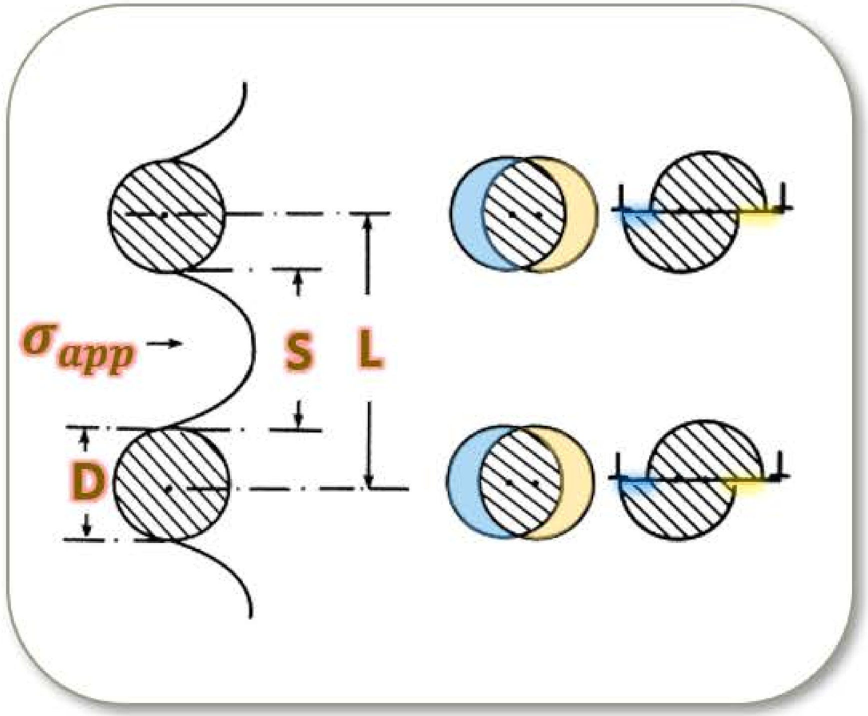


Wang D. et al., 2022. Journal of Nuclear Materials 569 153940

Nanovoids Influence Strengthening



Lucas G., 1993. Journal of Nuclear Materials 206 287-305

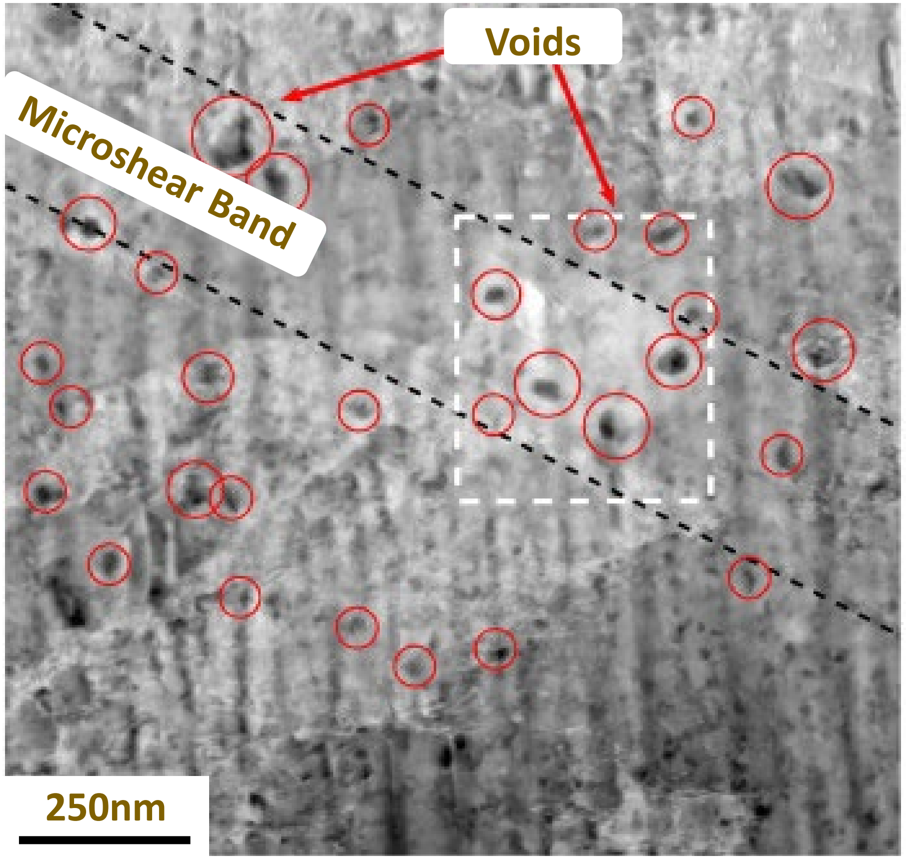


Precipitate Hardening Analog

Weak Obstacle

Influence Extends Beyond Irradiation Damage

Nanovoids Also Exist in Ductile Metals More Broadly…



Noell P. et al., 2020. Acta Mater. 184 211-224

Nanovoid Strengthening Literature

Irradiated Materials

Nanovoid Strengthening Literature

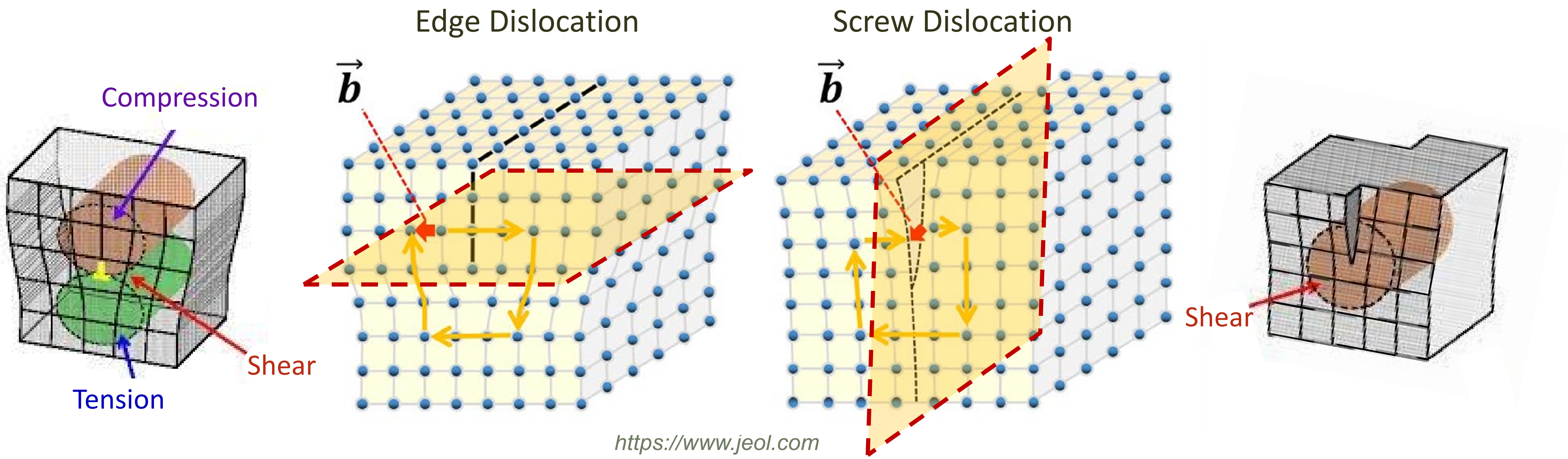
Simulation Approach with PFDD

Nanovoid Strengthening Trends

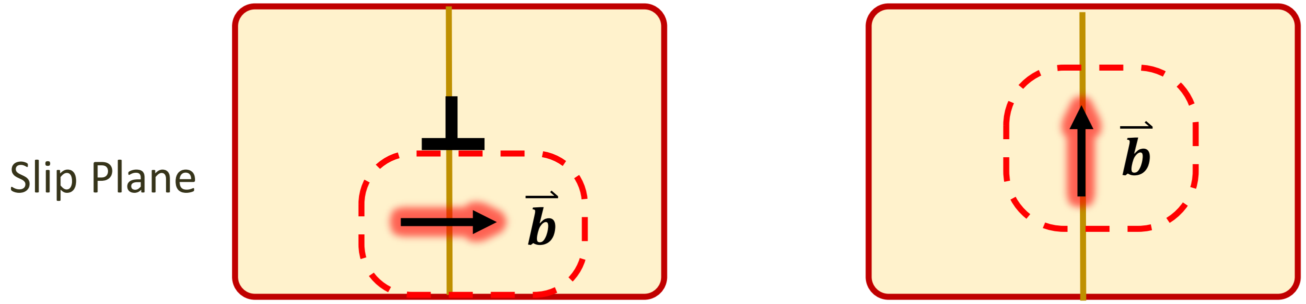
Dominant Mechanisms

Crash Course on Dislocation Mechanics

Dislocation Defects are Primary Carriers of Plastic Deformation



https://www.jeol.com

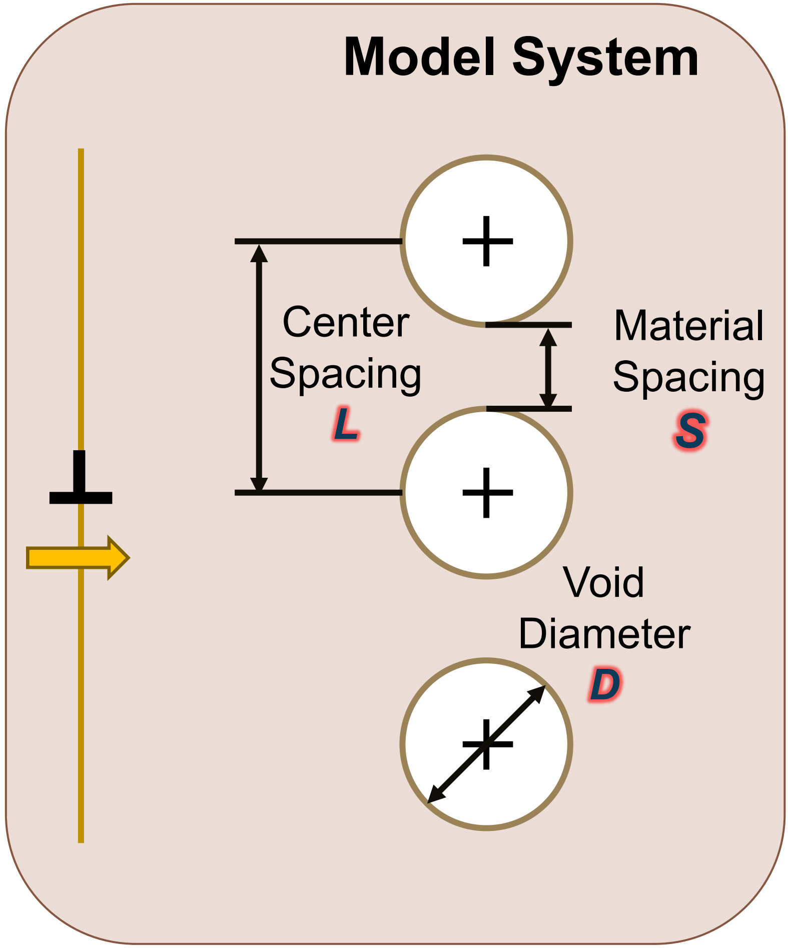


A few Angstrom ($10^{-10}m$) →

Avalanche of Millions to get

Macroscopic Deformation

Model System Analogous to Precipitate Hardening

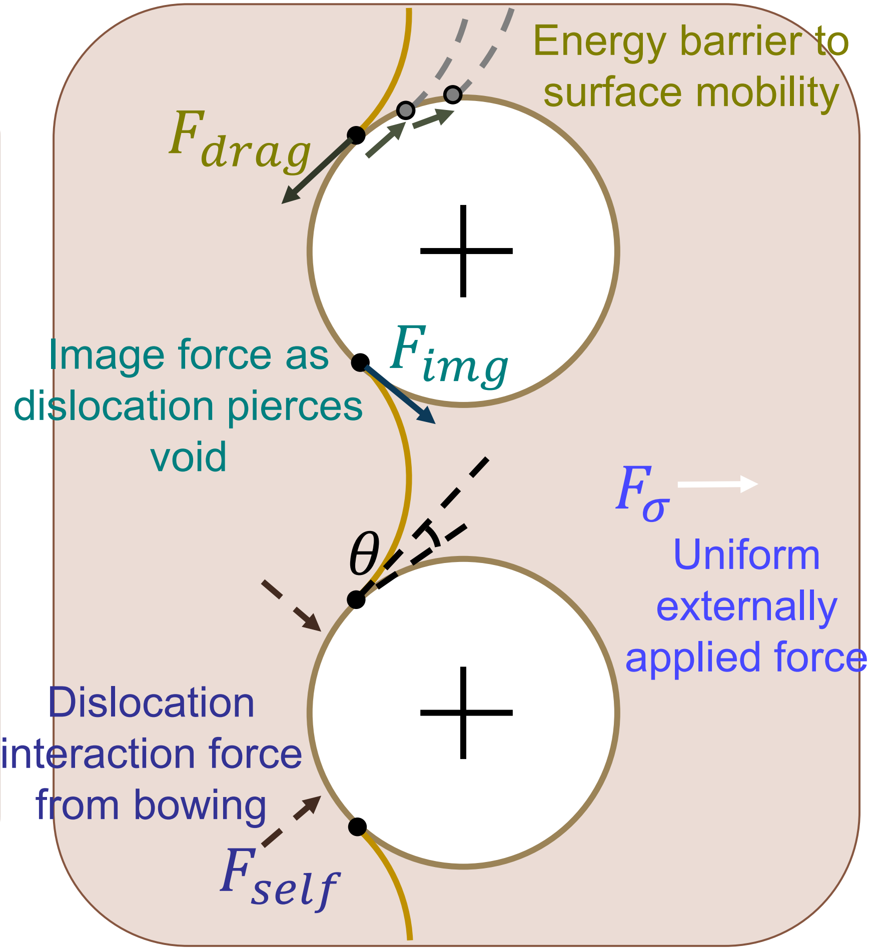


Model System

Center Spacing **L**

Material Spacing **S**

Void Diameter **D**



Energy barrier to surface mobility

F_{drag}

Image force as dislocation pierces void

F_{img}

F_σ

Uniform externally applied force

θ

Dislocation interaction force from bowing

F_{self}

Scattergood and Bacon, 1982

$$\frac{\tau_c}{\mu} = \frac{b}{2\pi S}\left[ln\left(\frac{1}{b}\underbrace{\frac{DS}{D+S}}_{\bar{D}}\right) + \Delta\right]$$

Crone, Munday, and Knap, 2015

$$\frac{\tau_c}{\mu} = \frac{b}{2\pi\left({D}/{2} + S\right)} ln\left(\frac{\bar{D}}{b}\right)$$

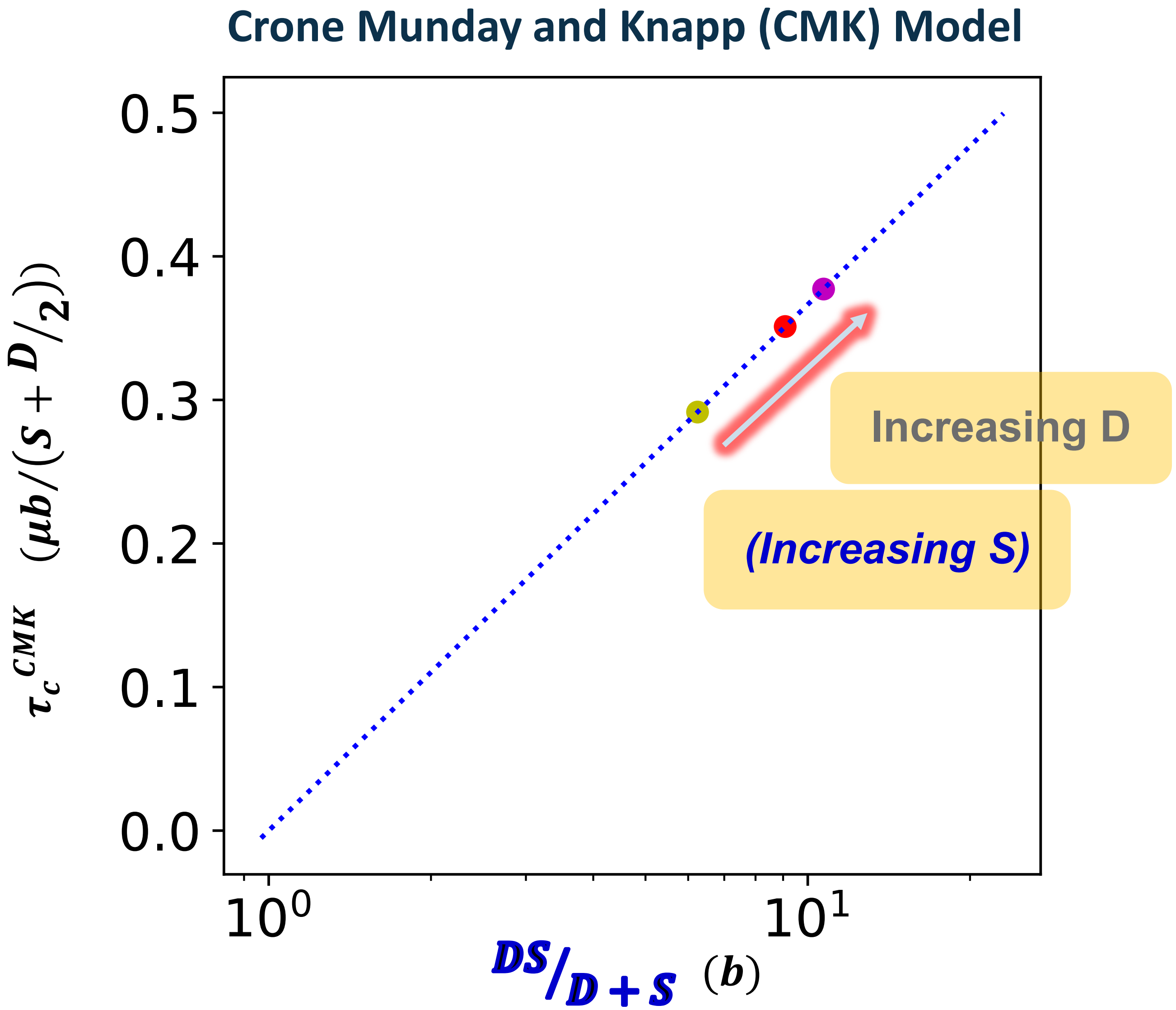
Obstacle: D, S, $\bar{D}$

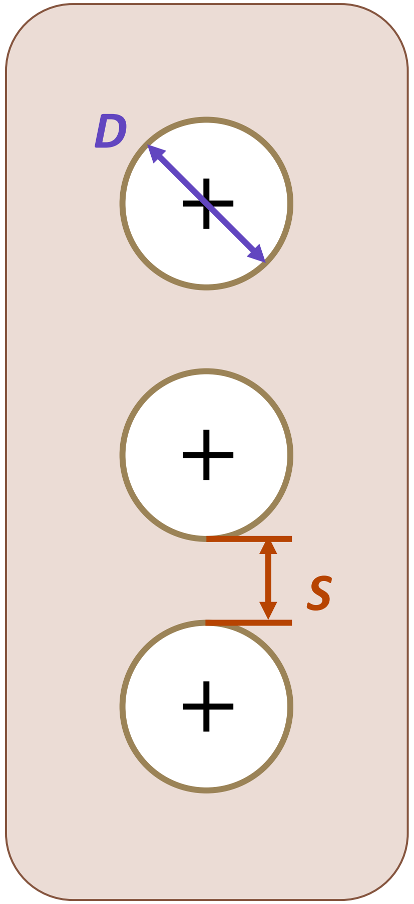
Material: b, μ

Scattergood R., Bacon D., 1982. Phil. Mag. 31 179-198

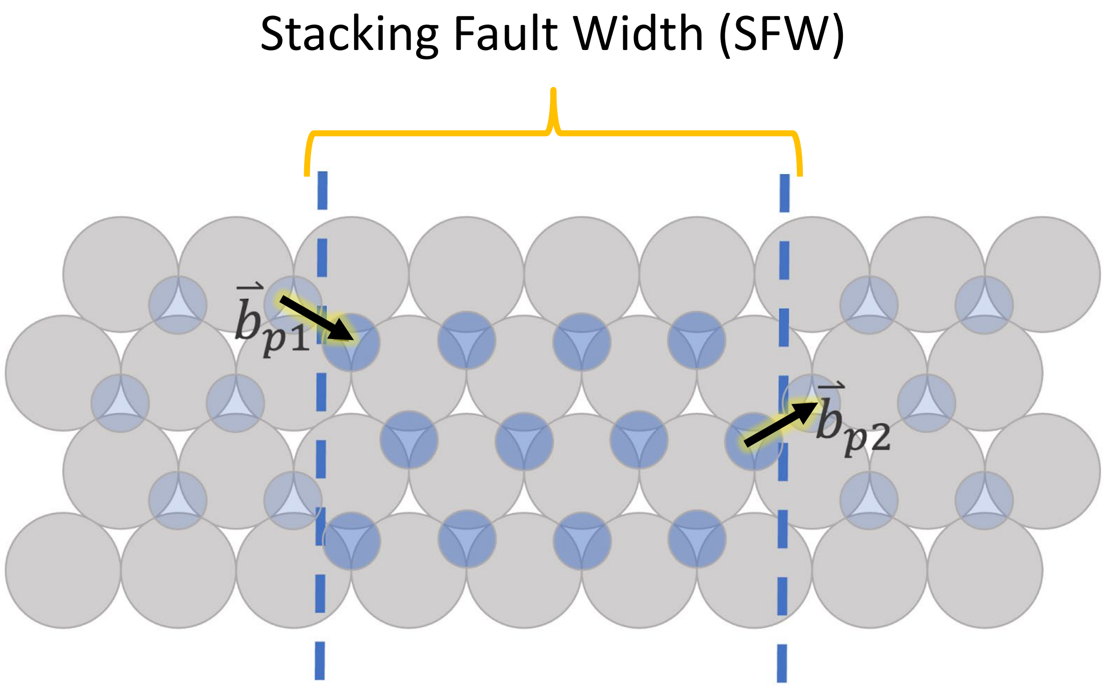
Crone J., Munday L., Knap J., 2015. Acta Mater. 101 40-47

Analytical Model Gives Complicated Strengthening Relationships



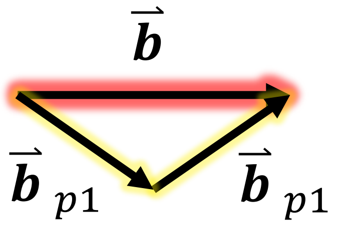


What About Dissociation in FCC Metals?



$$\frac{a}{2}[01\bar{1}] \rightarrow \frac{a}{6}[11\bar{2}] + \frac{a}{6}[\bar{1}2\bar{1}]$$

Separate Net Displacement into Partial Dislocation Steps

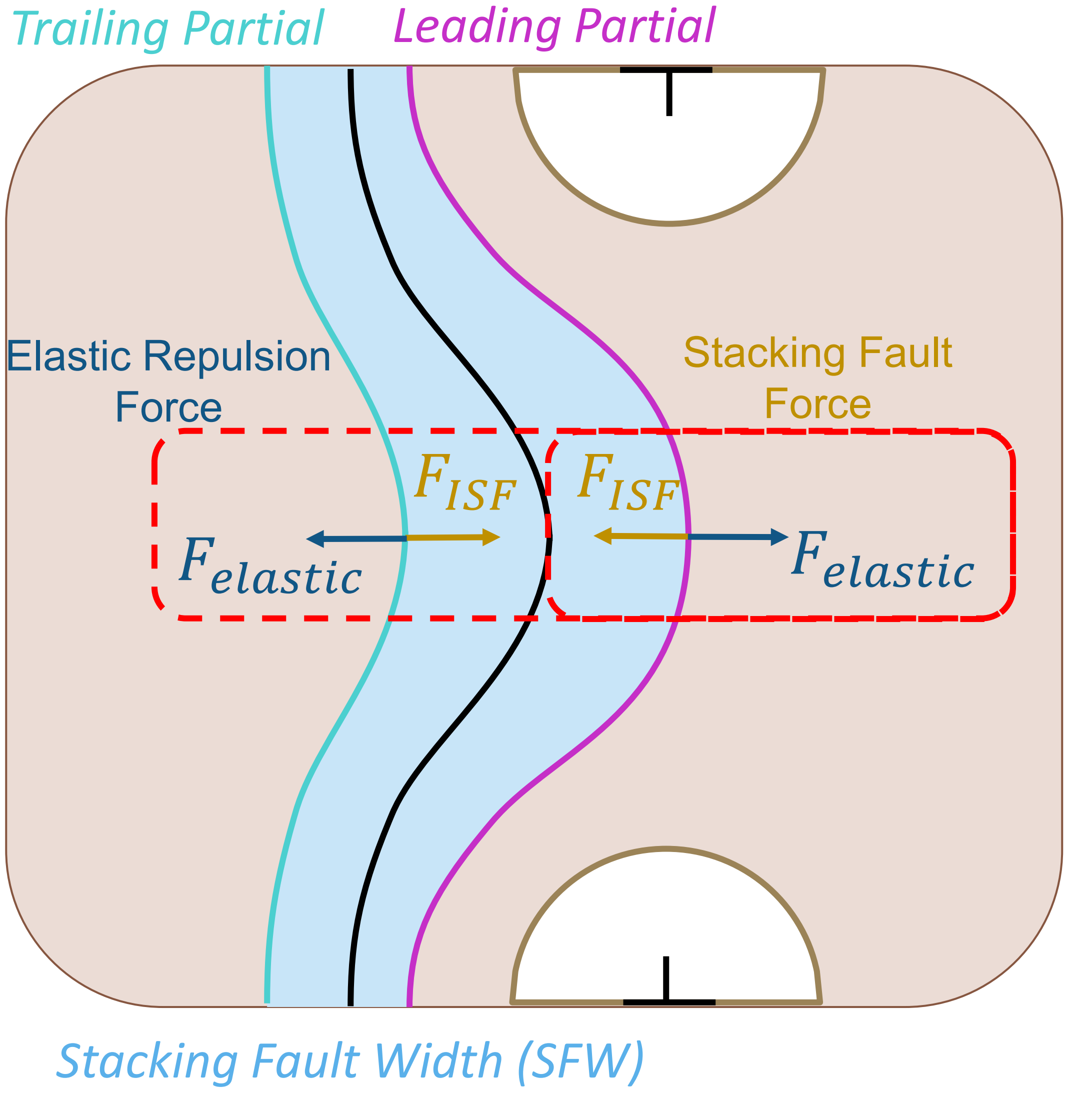


*Add Energetic Penalty with the **Stacking Fault***

*Change **Dislocation Character** for Each Partial*

*Lower **Line Tension** for Each Partial*

Dislocation Dissociation Alters the Fundamentals



If Partials Act Together:

Total Force Balance Remains Consistent ✓

If Partials Act Sequentially:

Total Force Balance Changes (!)

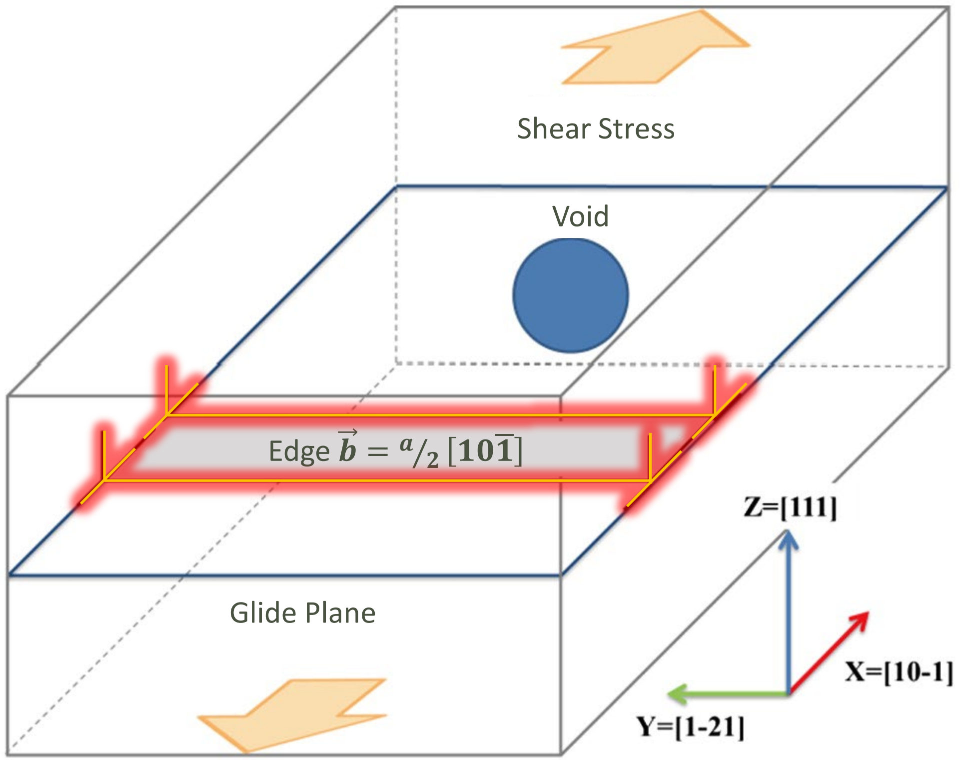
Larger SFW Materials

↓

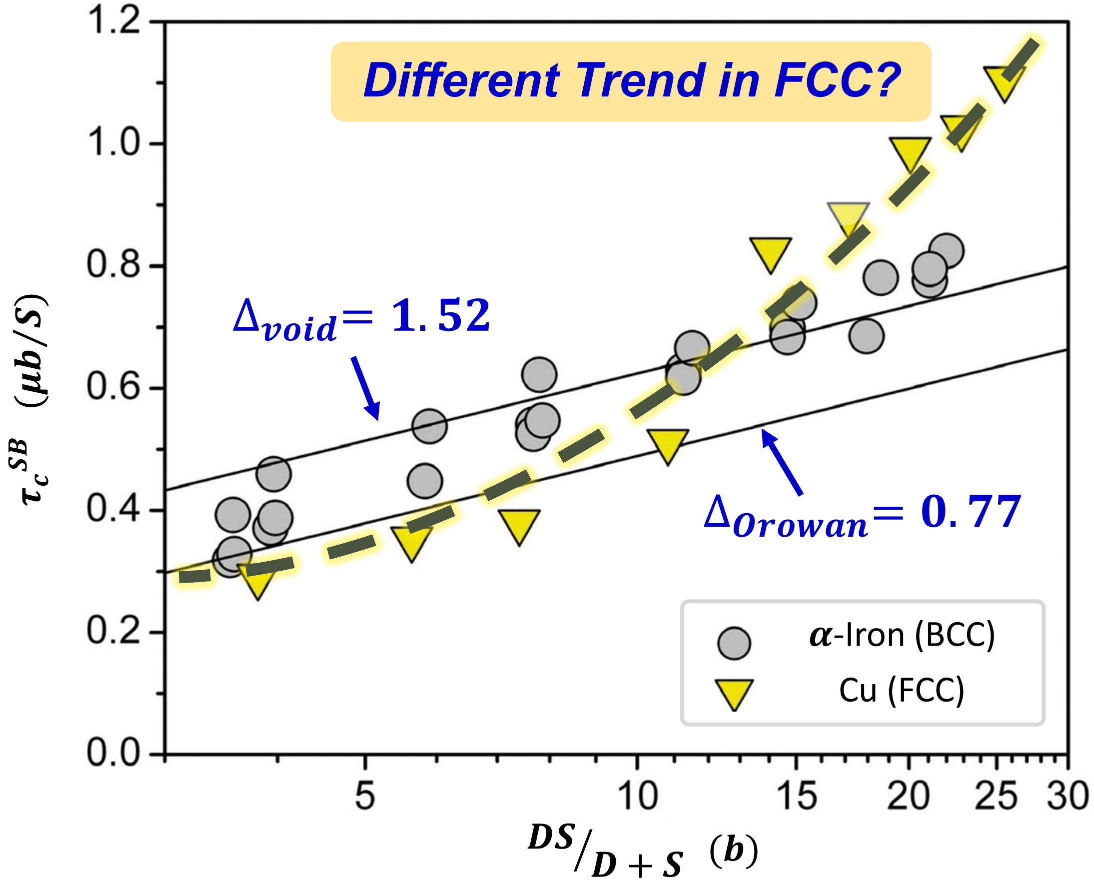
Higher Likelihood of Sequential Shearing

Extension to Partials in FCC and Atomistics

Atomistics Capture Dissociated Core



Strength Trends in MD versus Analytics



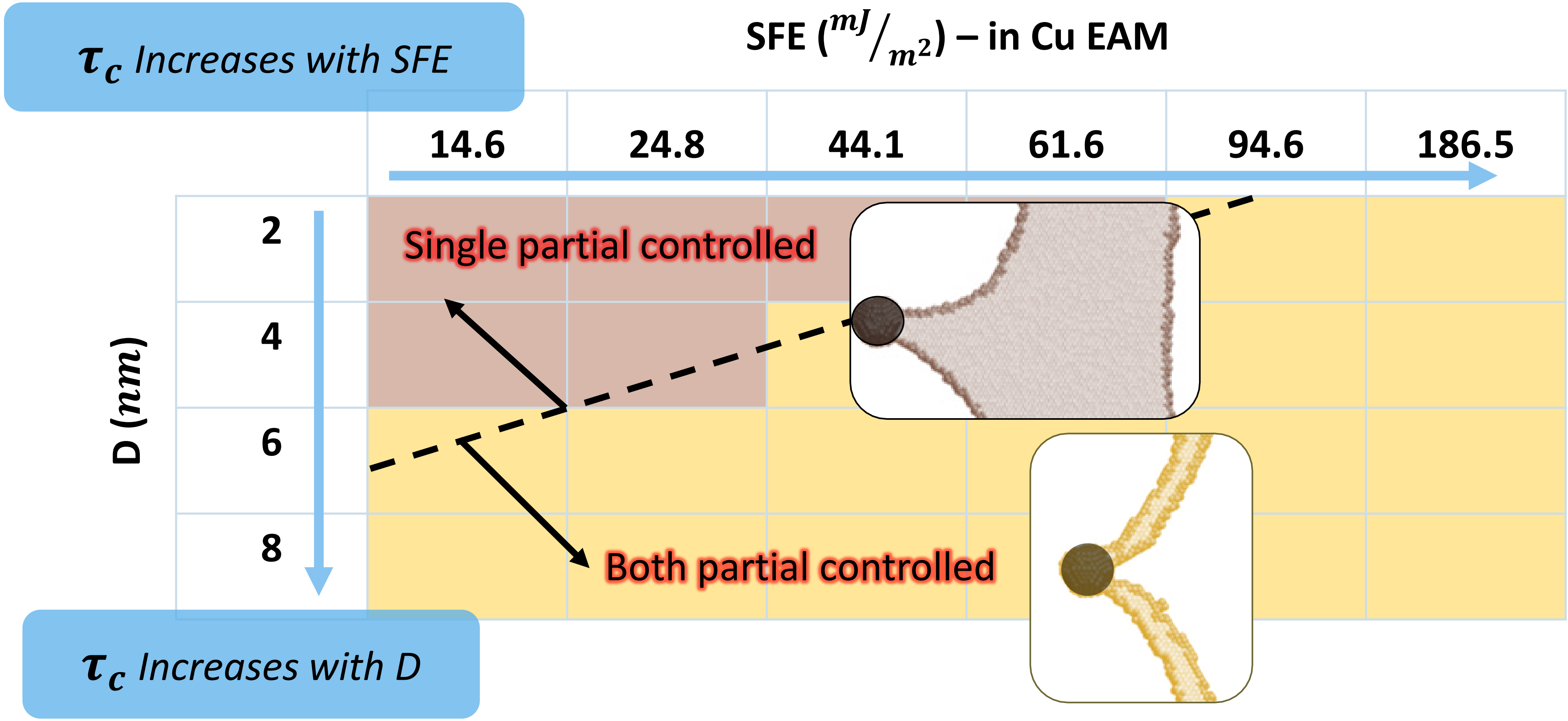
$$\frac{\tau_c^{SB}}{\mu} = \frac{b}{2\pi S}\left[ln\left(\frac{1}{b}\frac{DS}{D+S}\right) + \Delta\right]$$

Doihara K. et al., 2018. Phil. Mag. 98 2061-2076

Osetsky Y., Bacon D., 2010. Phil. Mag. 90 945-961

Size and Material Sensitivities are Expected

Pseudo-SFE Study into Material Dependence



$\boldsymbol{\tau_c}$ *Increases with SFE*

SFE ($^{mJ}/_{m^2}$) – in Cu EAM

$\boldsymbol{\tau_c}$ *Increases with D*

Asari K. et al., 2013. J. Nuclear Materials 442 360-364

Doihara K. et al., 2018. Phil. Mag. 98 2061-2076

Simar A., Voigt H.J.L., Wirth B.D., 2011. Comp. Material Sci. 50 1811-1817

Osetsky Y., Bacon D., 2010. Phil. Mag. 90 945-961

Additional Modeling Techniques Are Needed

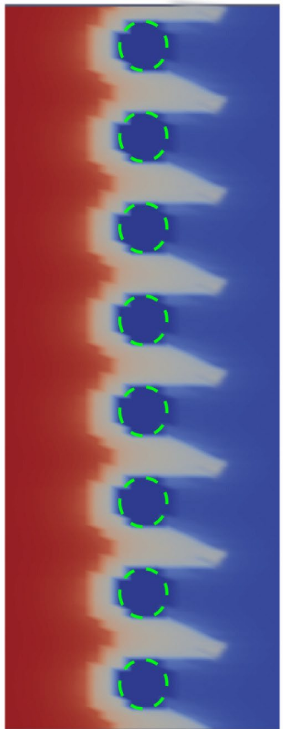
Molecular Dynamics (MD)		**Desired Metrics**
Small Void and Cell Sizes	✗	*Relevant **Length** Scales*
Shock Loading	✗	*Relevant **Time** Scales*
Limited Reliable Interatomic Potentials	✗	*Full **Material** Variability*

Nanovoid strengthening in FCC still has unanswered questions…

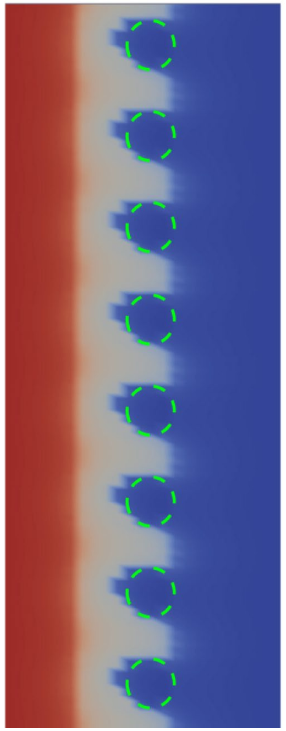
Phase Field Dislocation Dynamics (PFDD)

Energetic Framework: *Evolve* ***order parameters*** *and minimize* ***system energy*** *using* ***Time Dependent Ginzburg Landau (TDGL) Equation***

Unshearable Voids

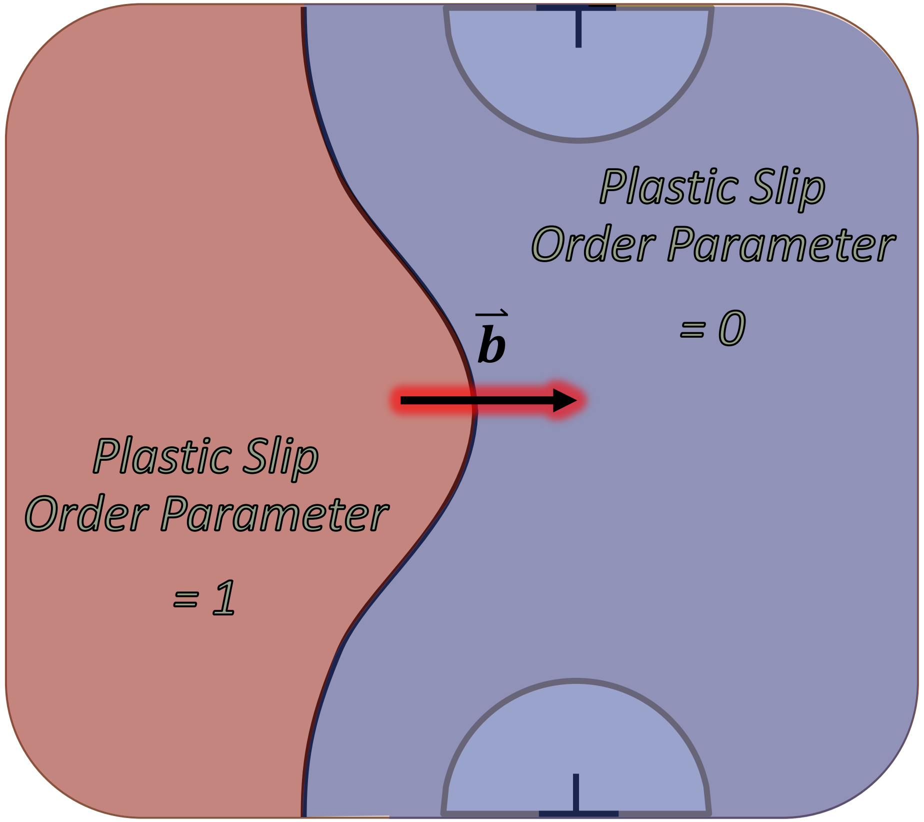


Shearable Pseudo-Voids



Xu S. et al., 2022. Comput. Meth. Appl. Mech. Eng. 389 114426

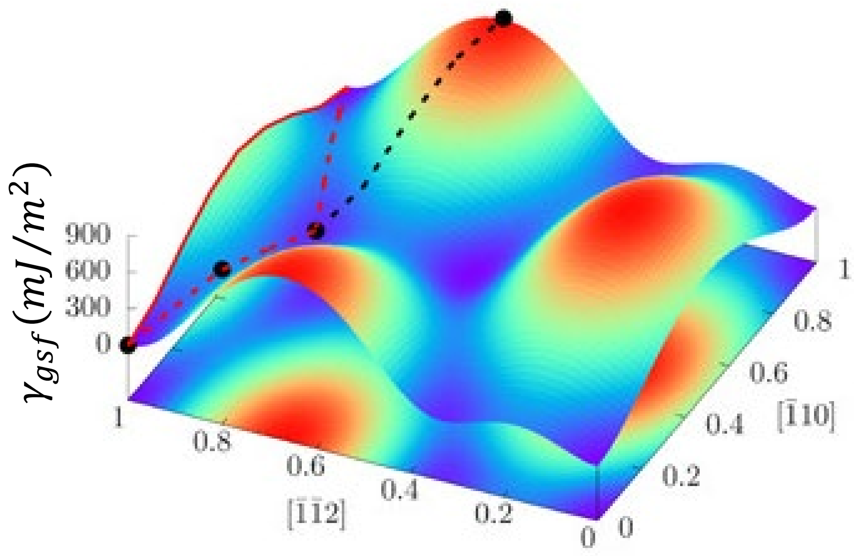
Dislocations as Boundaries Between *Slipped* and *Unslipped*



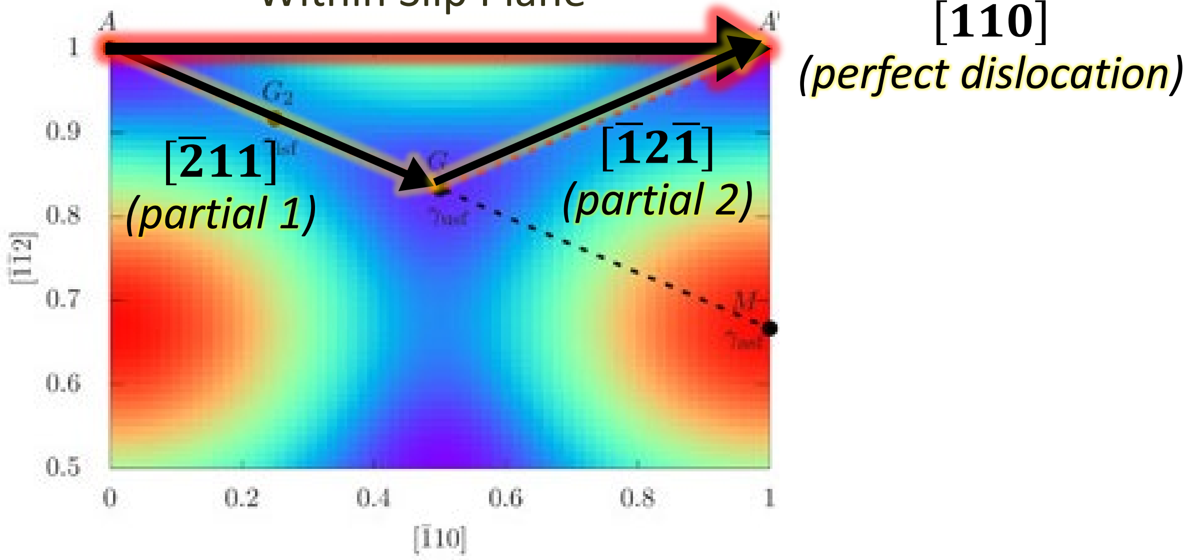
Gamma Surface Enables Physics-Driven Dislocation Evolution

Energetic Penalty to Dislocation Motion

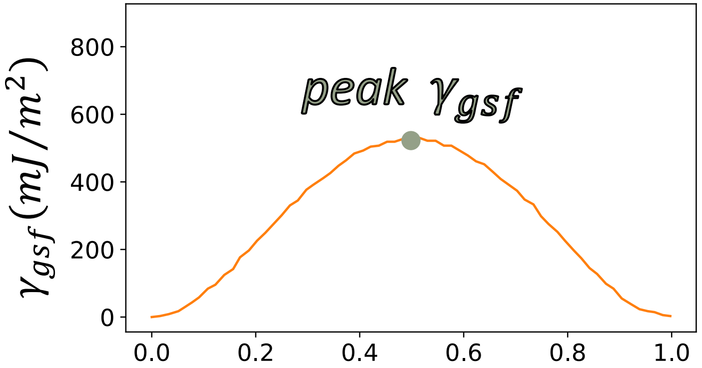
Energy Landscape



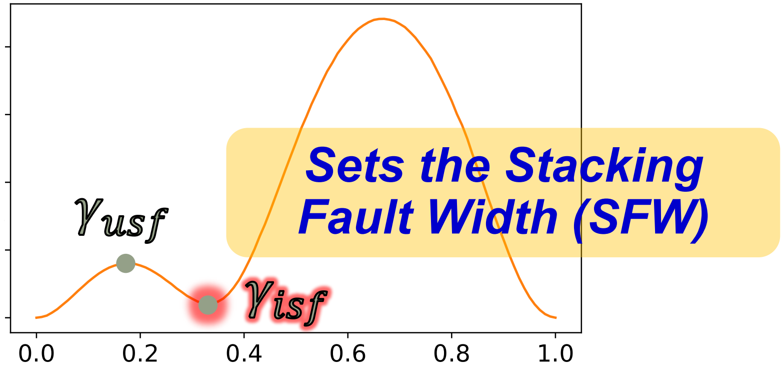
Within Slip Plane



GSFE Curve Along $[\bar{1}10]$



GSFE Curve Along $[\bar{2}11]$



Sets the Stacking Fault Width (SFW)

Enables Capture of Dissociation Physics Within Continuum Framework

Su et al./Journal of Applied Physics 126, 105112 (2019)

PFDD Expands our Investigative Abilities for this Problem

Phase Field Dislocation Dynamics (PFDD)		**Desired Metrics**
*Larger** *Cell Sizes* **(still small)*	✓	*Relevant **Length** Scales*
Stress Controlled Motion	✓	*Relevant **Time** Scales*
Easily Probe SFE Space • *Elastic Anisotropy* • *Material Inhomogeneity* • *Gamma Surfaces*	✓	*Full **Material** Variability*

Simulation Approach:
Phase Field Dislocation Dynamics (PFDD)

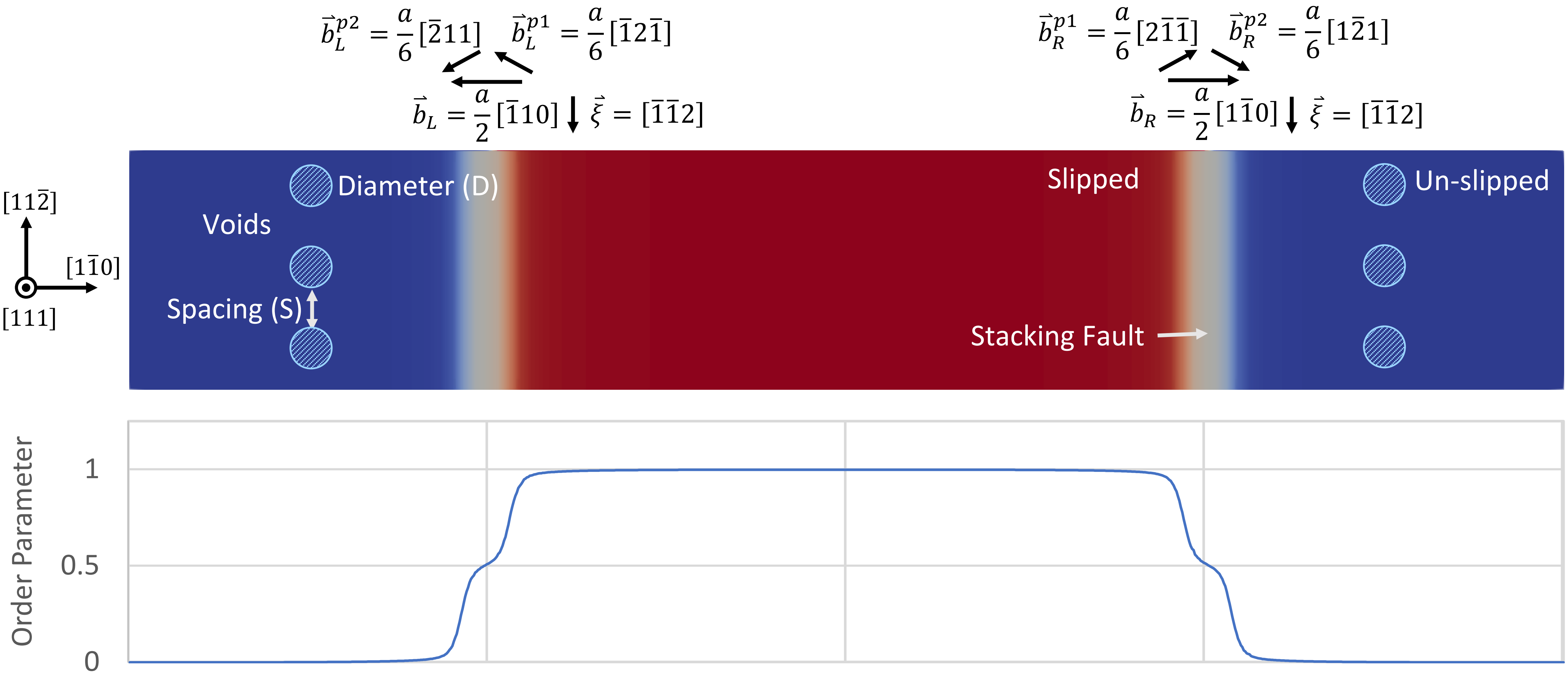
- Irradiated Materials
- Nanovoid Strengthening Literature
- **Simulation Approach with PFDD**
- Nanovoid Strengthening Trends
- Dominant Mechanisms

Simulation Cell Design for Voids in PFDD

Perfect Dislocation Dipole

Periodic boundaries in x, y, z

Simulation Cell Design for Voids in PFDD



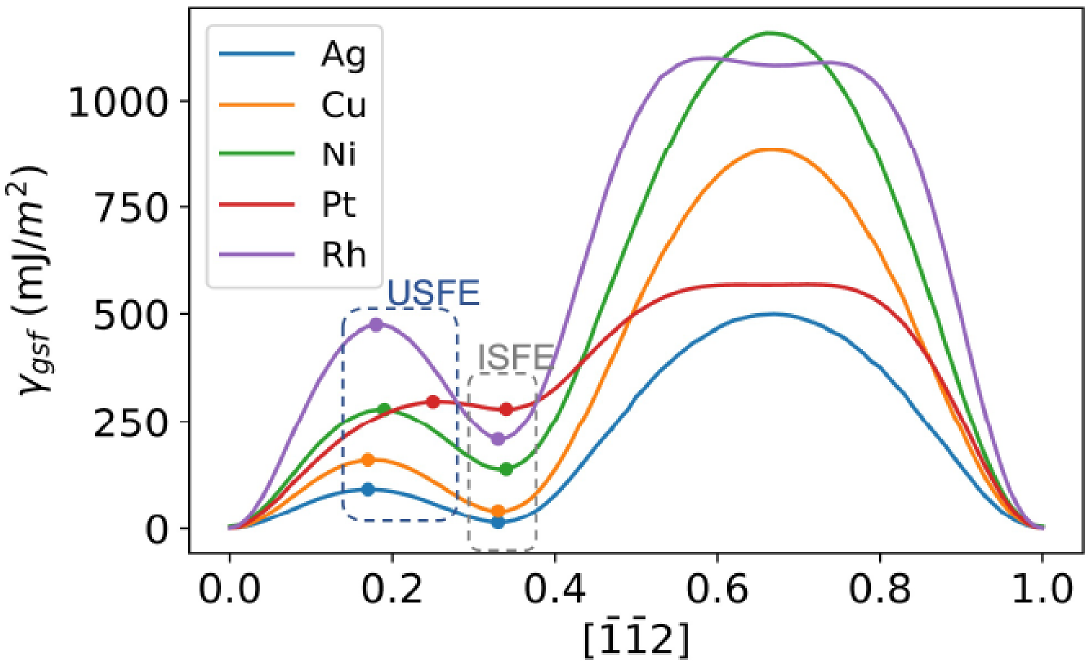
$\vec{b}_L^{p2} = \frac{a}{6}[\bar{2}11]$ $\vec{b}_L^{p1} = \frac{a}{6}[\bar{1}2\bar{1}]$

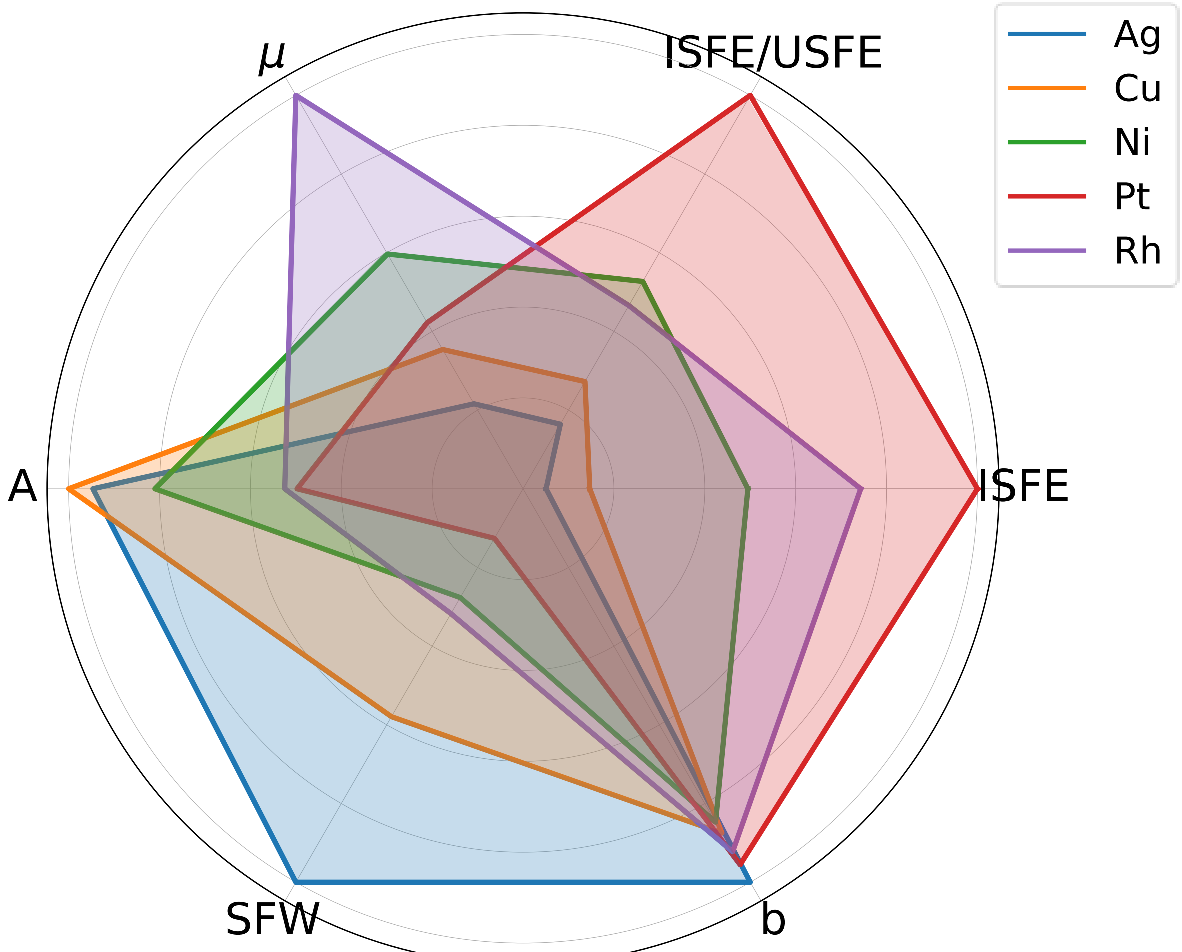
$\vec{b}_L = \frac{a}{2}[\bar{1}10]$ ↓ $\vec{\xi} = [\bar{1}\bar{1}2]$

$\vec{b}_R^{p1} = \frac{a}{6}[2\bar{1}\bar{1}]$ $\vec{b}_R^{p2} = \frac{a}{6}[1\bar{2}1]$

$\vec{b}_R = \frac{a}{2}[1\bar{1}0]$ ↓ $\vec{\xi} = [\bar{1}\bar{1}2]$

Material Inputs Consider All Properties

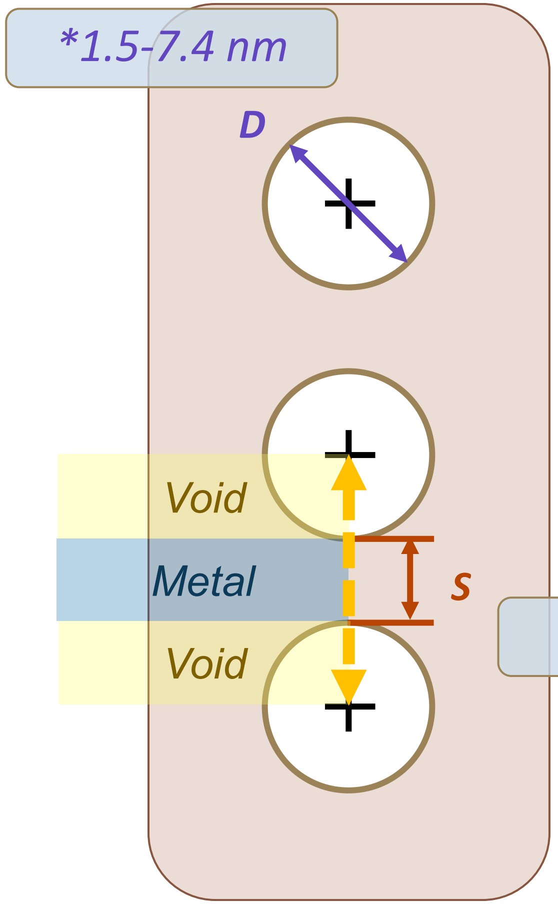




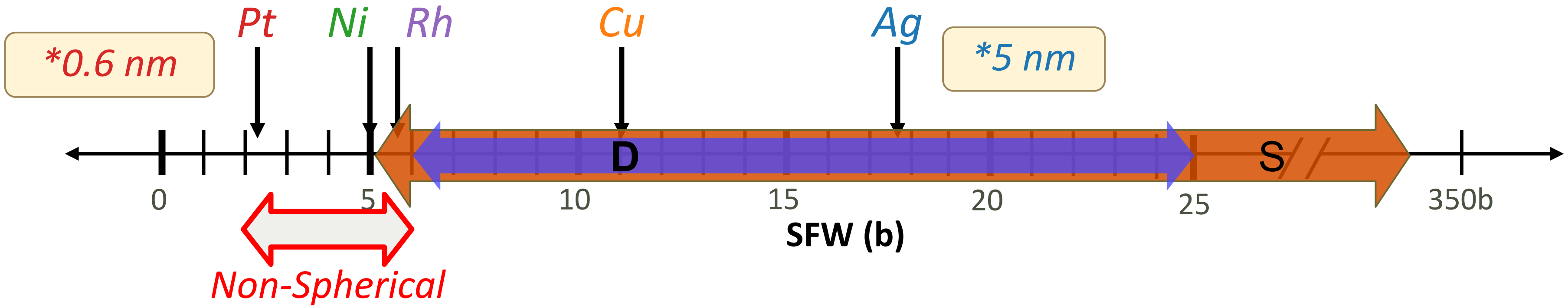
Material	ISFE/USFE
Silver	0.15
Copper	0.26
Rhodium	0.44
Nickel	0.50
Platinum	0.94

more diffuse core than dissociated core

Void Geometries Span Characteristic Lengths



*1.3-93 nm



Alternative Geometry Parameter:

Linear Void Fraction

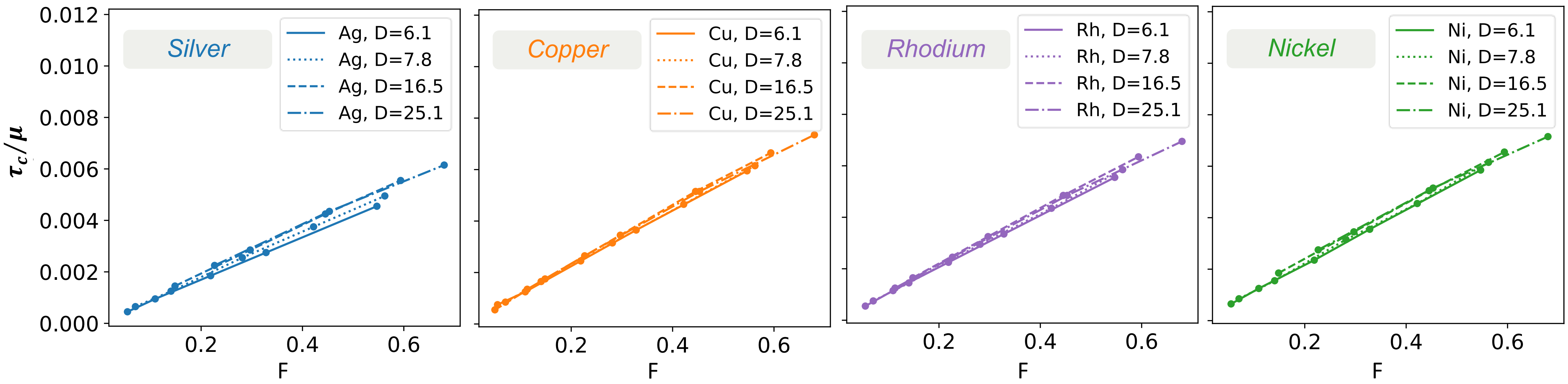
$$F = \frac{D}{D+S}$$

Local Obstacle Density

$$5\% \leq F \leq 70\%$$

Results: Nanovoid Strengthening Trends

Strong Dependence on Linear Void Fraction



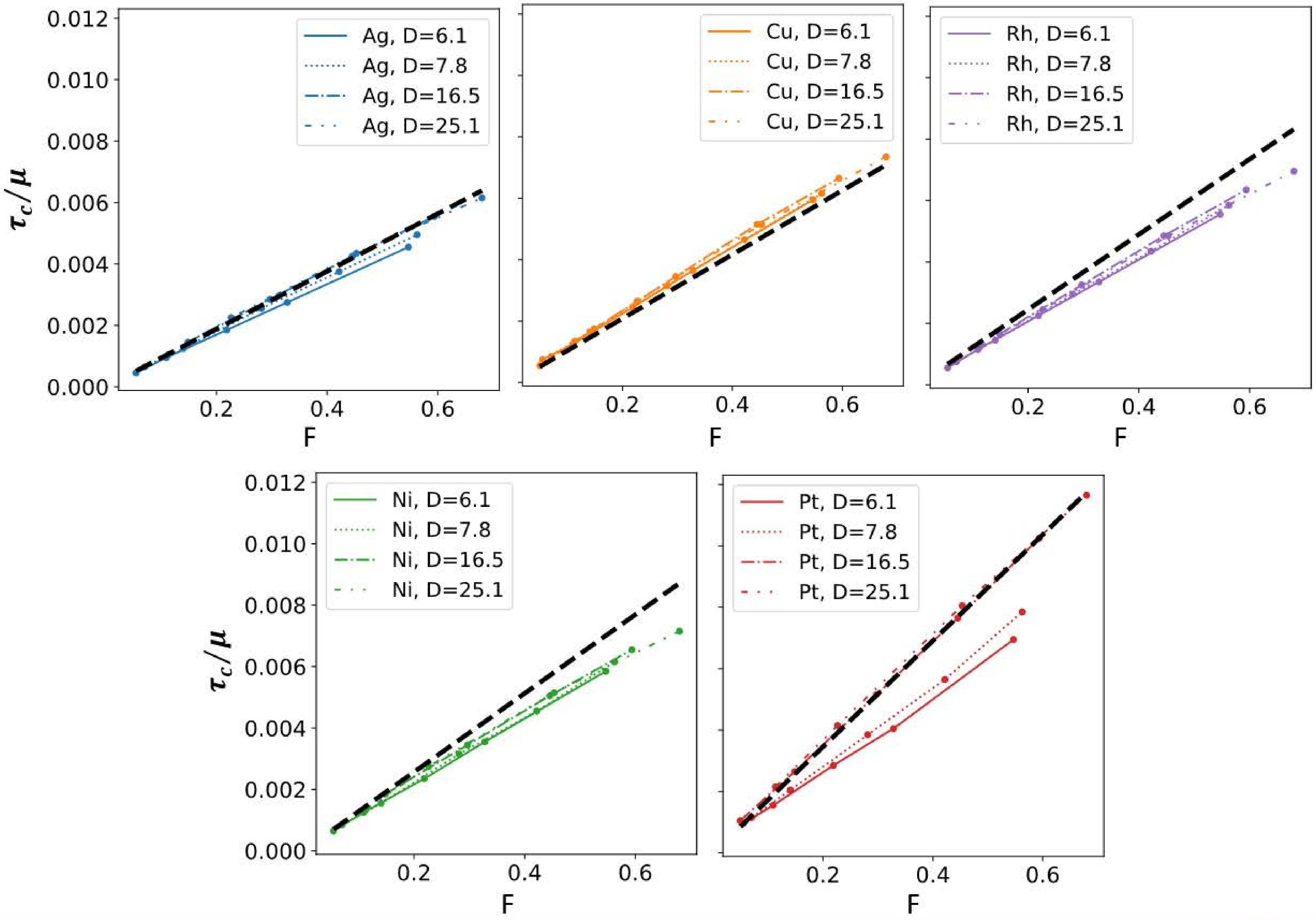
Remarkable collapse to single curve for τ_c/μ *versus F*

no higher order D or S dependence

Strong $\boldsymbol{\mu}$ *dependence*

ISFE/USFE is a Dominant Property

$$\frac{\tau_c}{\mu} = \left(\frac{\frac{ISFE}{USFE} + \frac{\pi}{4}}{100} \right) F$$



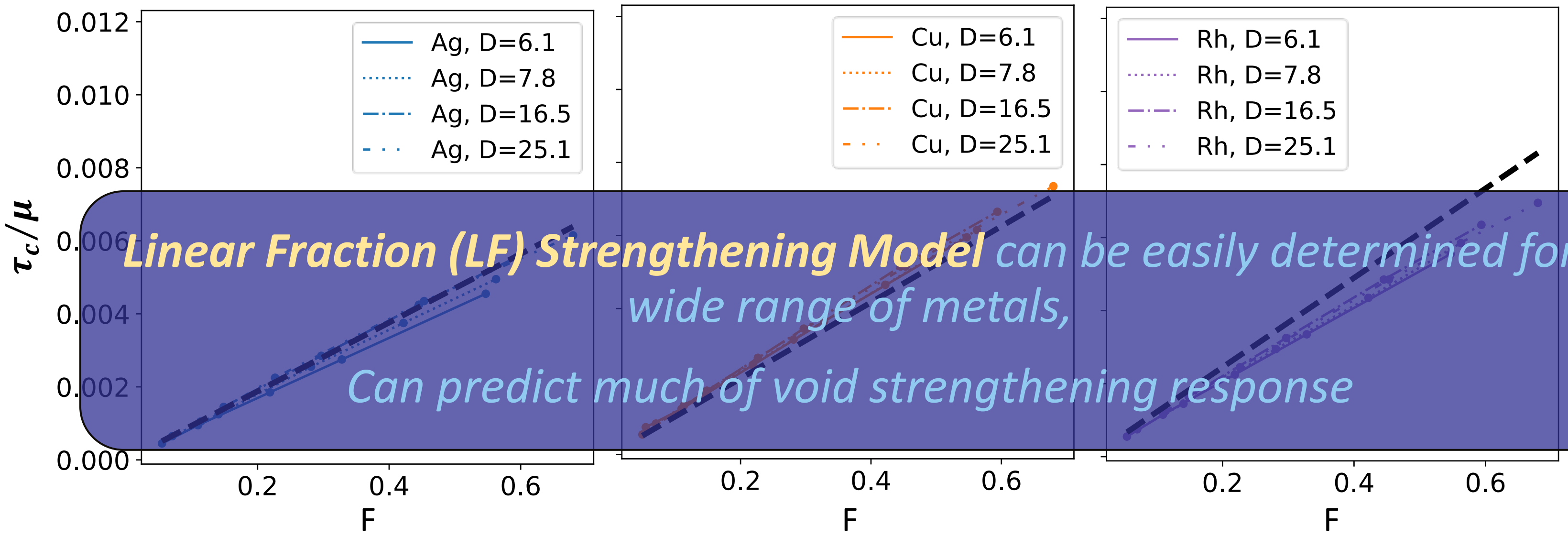
Material Ranking

PFDD	*Equation*
Ag	Ag
Rh	
Ni	Rh
	Ni
Pt	Pt

τ_c

ISFE/USFE is a Dominant Property

$$\frac{\tau_c}{\mu} = \left(\qquad \right)_F$$



Linear Fraction (LF) Strengthening Model *can be easily determined for wide range of metals,*

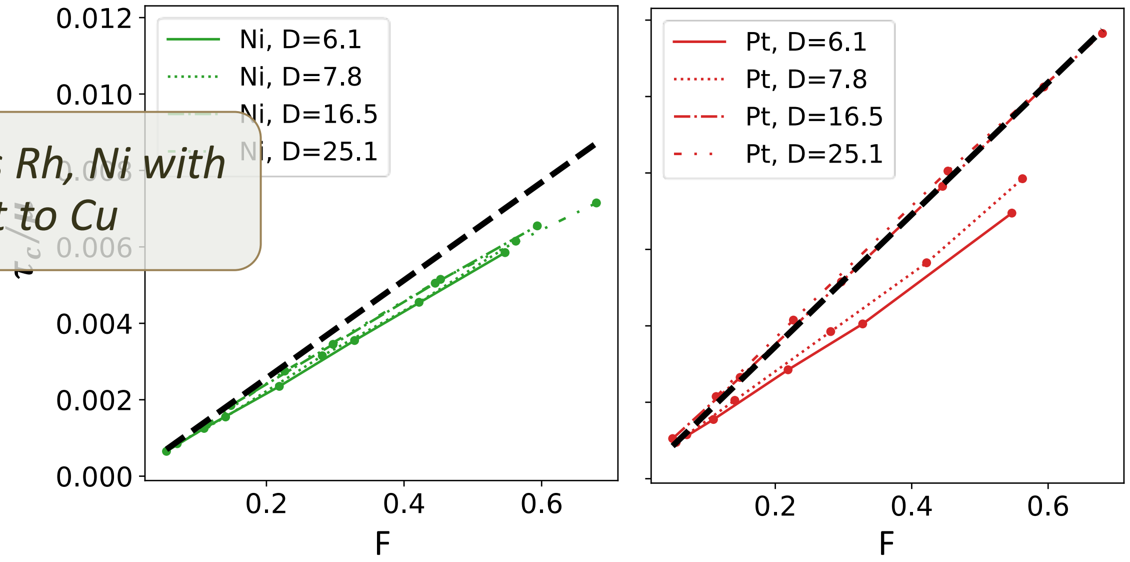
Can predict much of void strengthening response

Material Ranking

PFDD	*Equation*
Ag	Ag
Rh	Cu
Ni	Rh
Cu	Ni
Pt	Pt

τ_c

Overpredicts Rh, Ni with respect to Cu



Obstacle Strength Trends Shift from Literature

Strengthening Dependence from Literature

$$\frac{\tau_c}{\mu} = \frac{b}{2\pi L_{effective}} ln\underbrace{(S * F)}_{}$$

Logarithmic dependence on void geometry

Additional dependence on characteristic length at max bowing

Higher order void geometry dependence than F alone captures

Our LF Model

$$\frac{\tau_c}{\mu} = (M)F$$

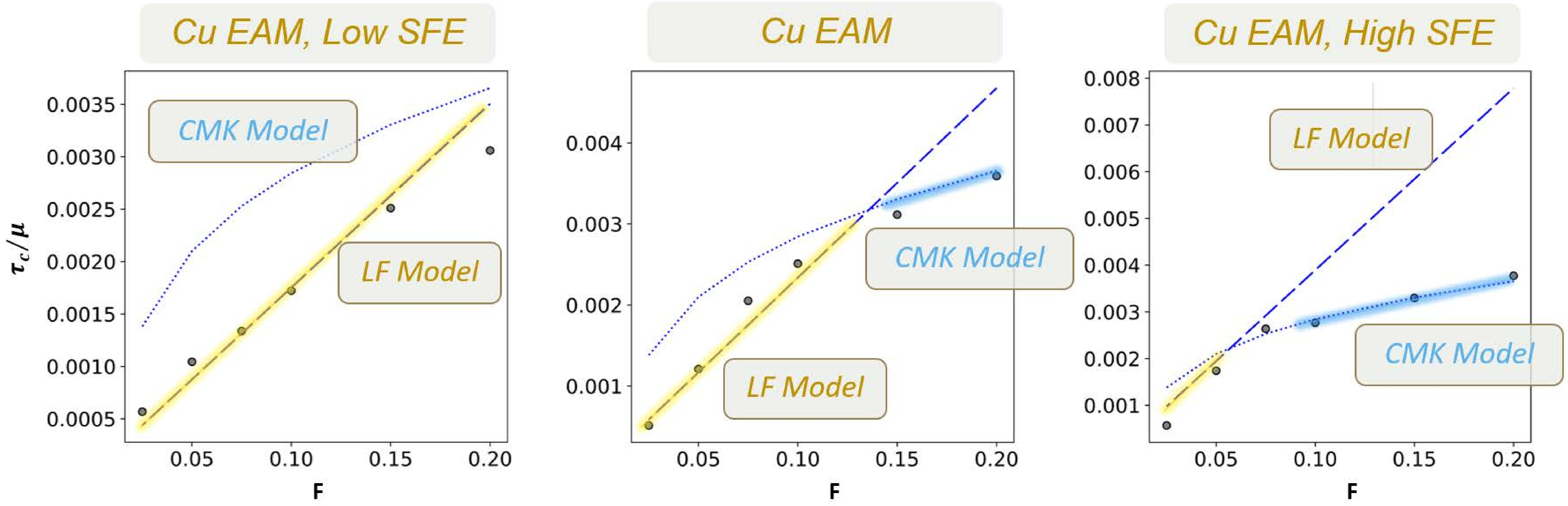
Linear dependence on void geometry

$$\frac{\tau_c}{\mu} = \alpha\left(\frac{ISFE}{USFE} + \beta\right)F$$

Empirical slope dependent ONLY on material properties

Relevance of Our LF Model in FCC Due to Dissociation

Comparing to Pseudo-SFE Study in MD



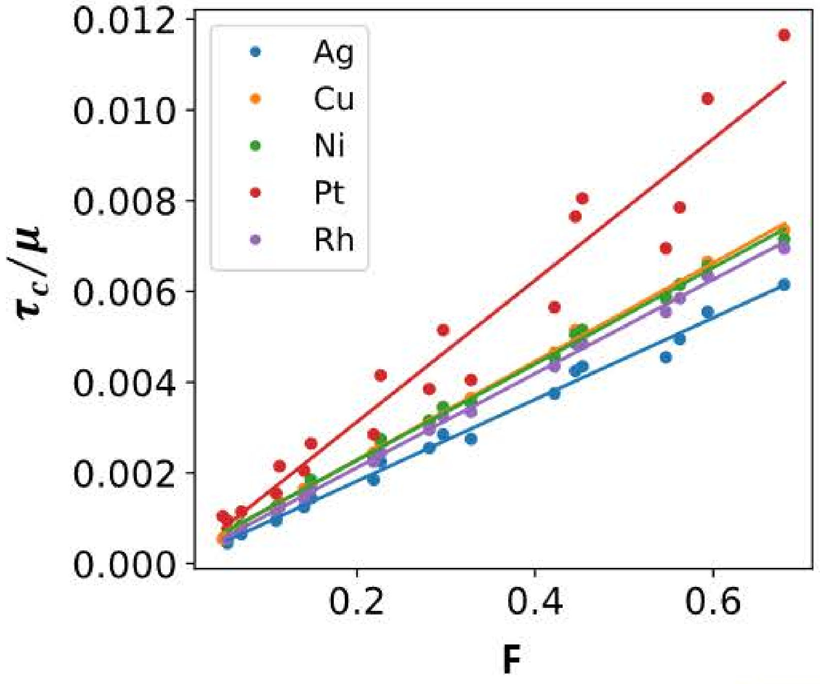
$$\frac{\tau_c^{LF}}{\mu} = \alpha\left(\frac{ISFE}{USFE} + \beta\right)F$$

$$\frac{\tau_c^{CMK}}{\mu} = \frac{b}{2\pi(S + D/2)} \ln\left(\frac{1}{b}\frac{DS}{D + S}\right)$$

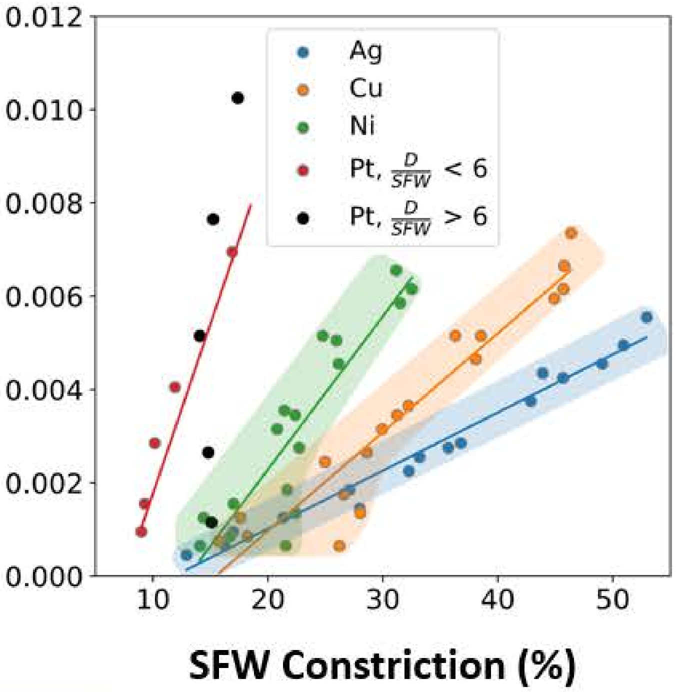
Asari K. et al., 2013. J. Nuclear Materials 442 360-364

Takeaways from Nanovoid Strengthening with PFDD

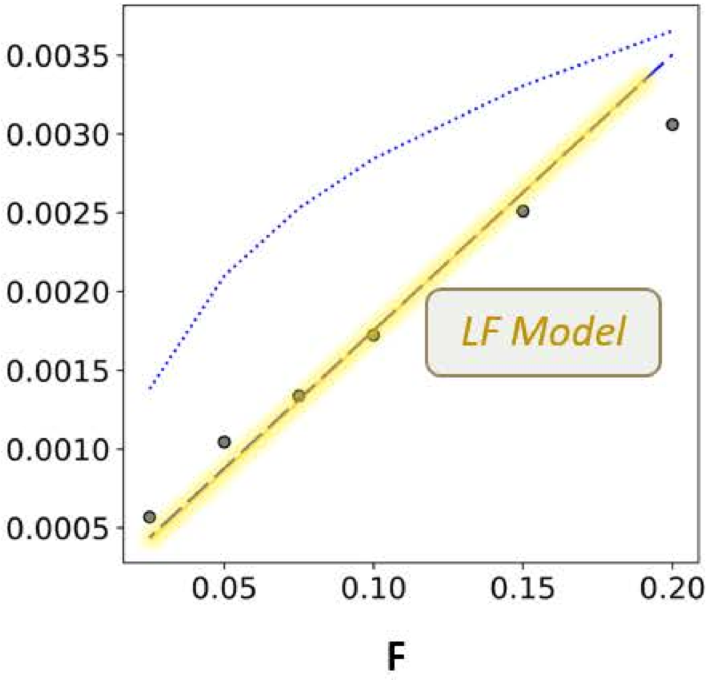
Linear Strengthening Curve in FCC



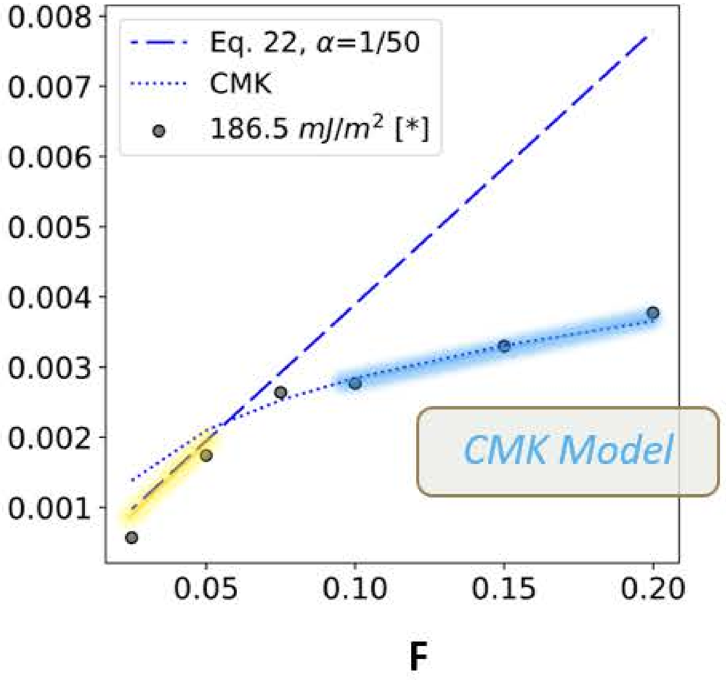
Dissociation Governs Response



LF Model Relevant for Low SFE Metals



Un-Dissociated Model Relevant for High SFE



$$\underbrace{\frac{\tau_c}{\mu} = \alpha\left(\frac{ISFE}{USFE} + \beta\right)F}_{\text{LF Model}}$$

Relevant Obstacle Dimensions: ~~D, S, $\bar{D}$~~ F

Relevant Material Properties: ~~b,~~ μ, $^{ISFE}/_{USFE}$