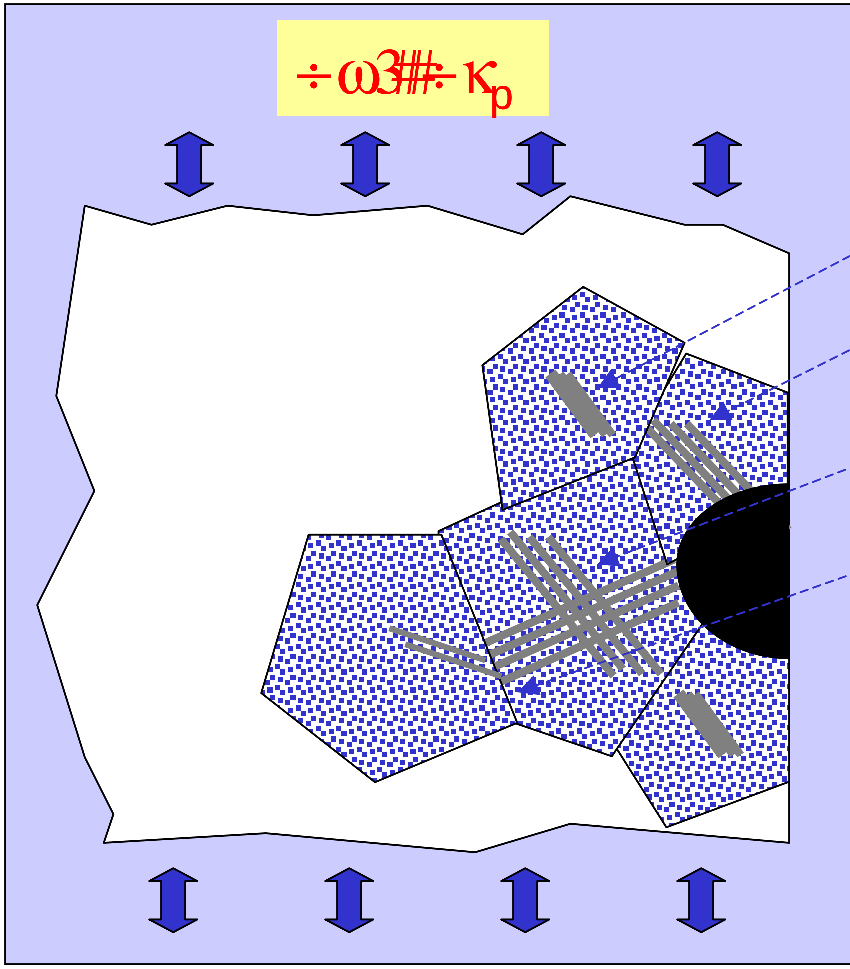
VISION : Predict Microstructure-Sensitive Cyclic ω4κ Curves !



σ4structure Sensitivity of Plasticity in MONOTONIC Loading

Slip Initiation : Source Strengths

Dislocation-Precipitate Interactions

Multislip Work-Hardening within Grain

Grain-Grain Interaction

Bridge with FATIGUE MODELS (McDowell, ..)

Cyclic Slip, Slip Localization

Key : Include as many Microstructural & Chemistry Variables as Possible

Report Documentation Page

Form Approved
OMB No. 0704-0188

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Standard Form 298 (Rev. 8-98)
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OUTLINE

Microstructure Effects Within Grains (ν2ν')

Using DD SIMULATIONS (S.Rao, T.A.Parthasarathy, D.M.Dimiduk, P.M.Hazzledine)

- PROGRESS : Established a Working Model / Methodology
- CURRENT FOCUS : Connectivity ("Handshakes")

Using FEM (Y-S Choi, T.A.Parthasarathy, D.M.Dimiduk)

- Unit Cell Model : Identified Key Issues - Refinements

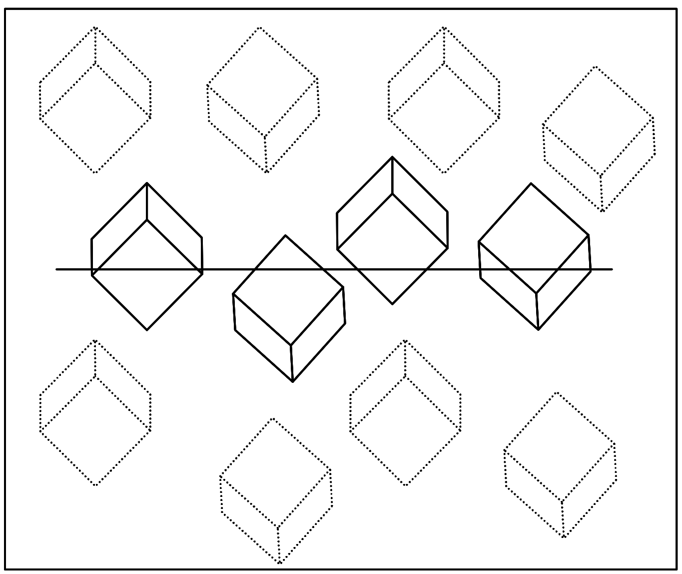
Grain-Grain Interaction

- Polycrystal Model : Using DD results

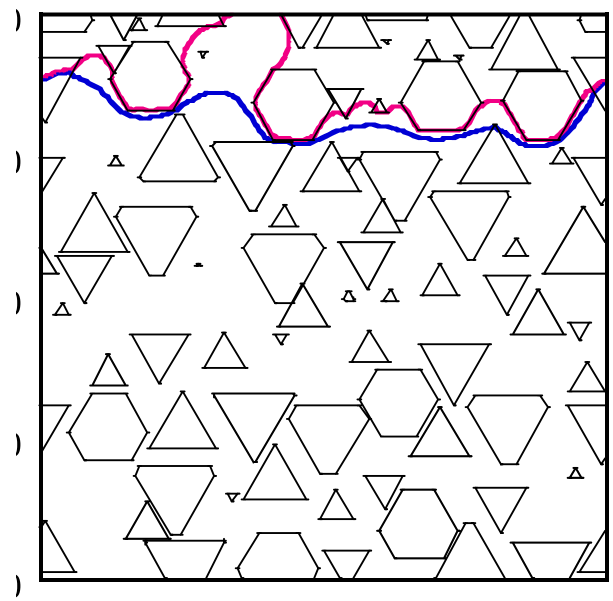
Grain-Defect Interaction

Discrete Dislocation (DD) Simulations

(111) Sections



Random Distribution of Cubes in a box



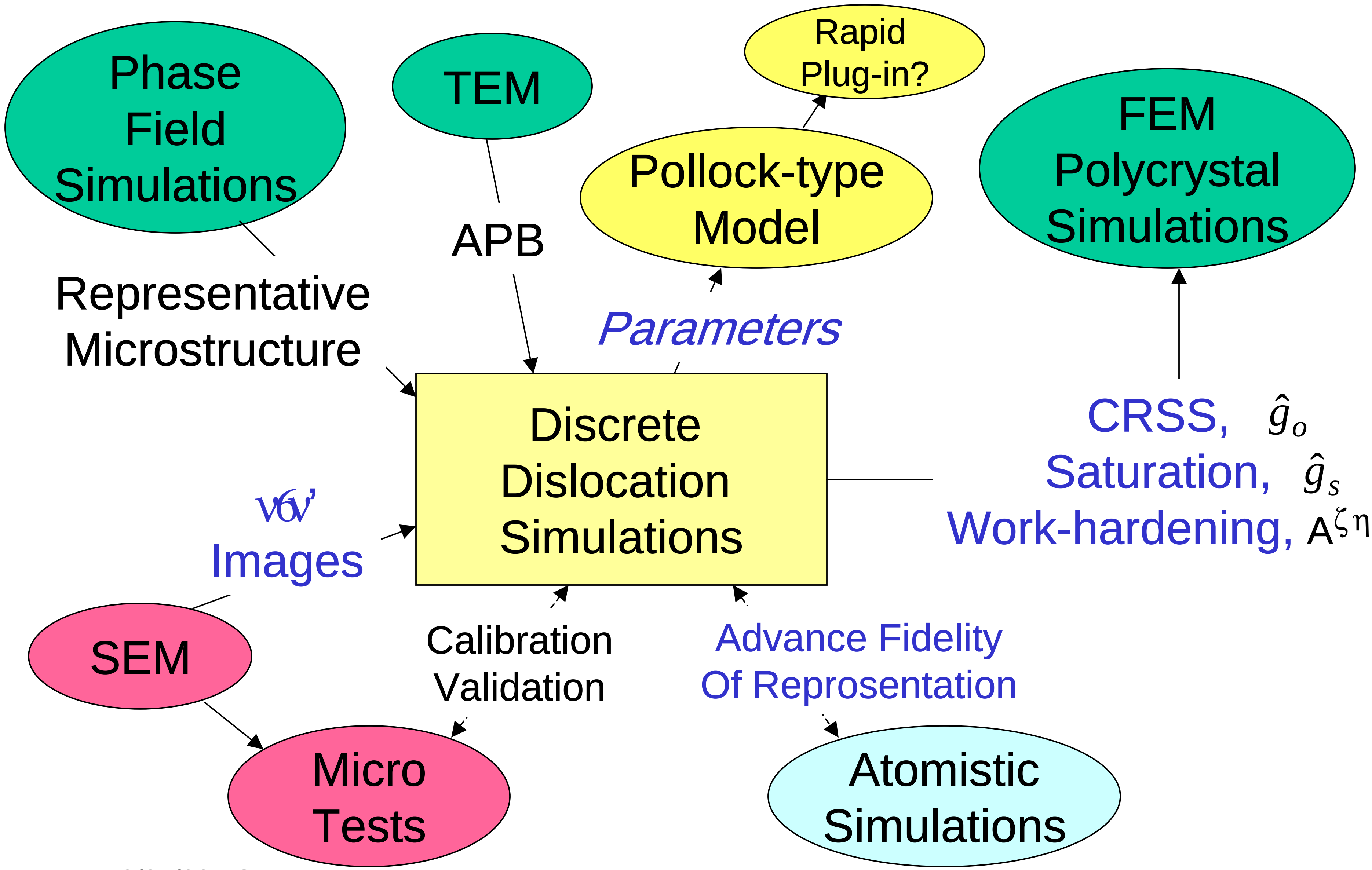
Spatial Distribution Varies with Plane of Sectioning

DD : Established 2D Methodology (Low T athermal)

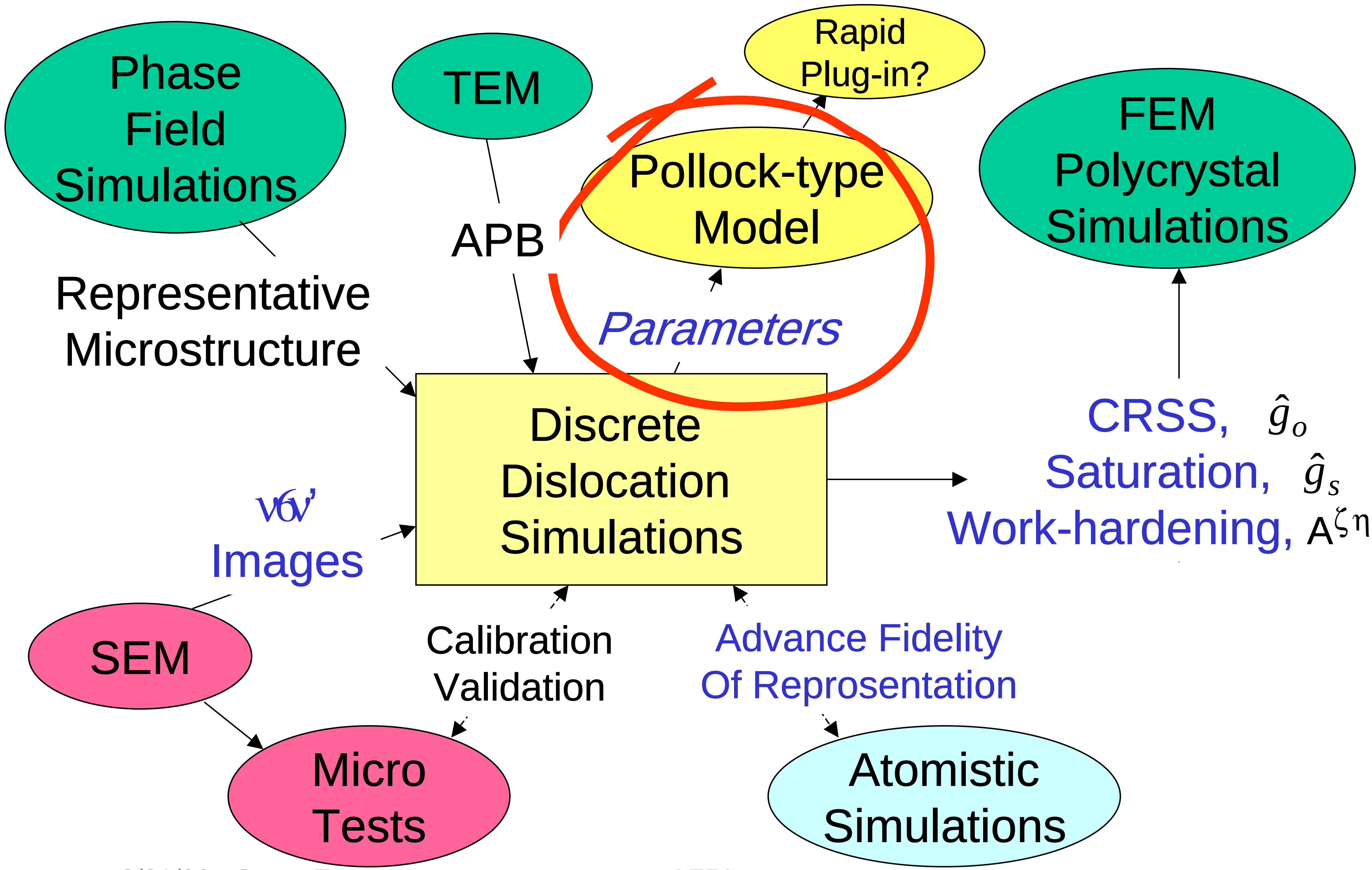
Model	Findings : Parametric Studies	Issues
Precipitate Hardening	Differs from Analytical Model (Reppich) Size & V_f Dep. Reasonable (Expt.) Real Microstructure Simulated	Other Models ? Scatter, ~10% Thresholding
	APB Energy : Primary Factor Friction Stress in ν Significant Coherency, Curvature : Negligible	Measure/Calc. Measure ?
Multi-Slip WH	3D with cross-slip (Comp. Limited)	Parallel Proc. (CHSSI, AFOSR)

Need "Handshakes" to Meet AIM Goals

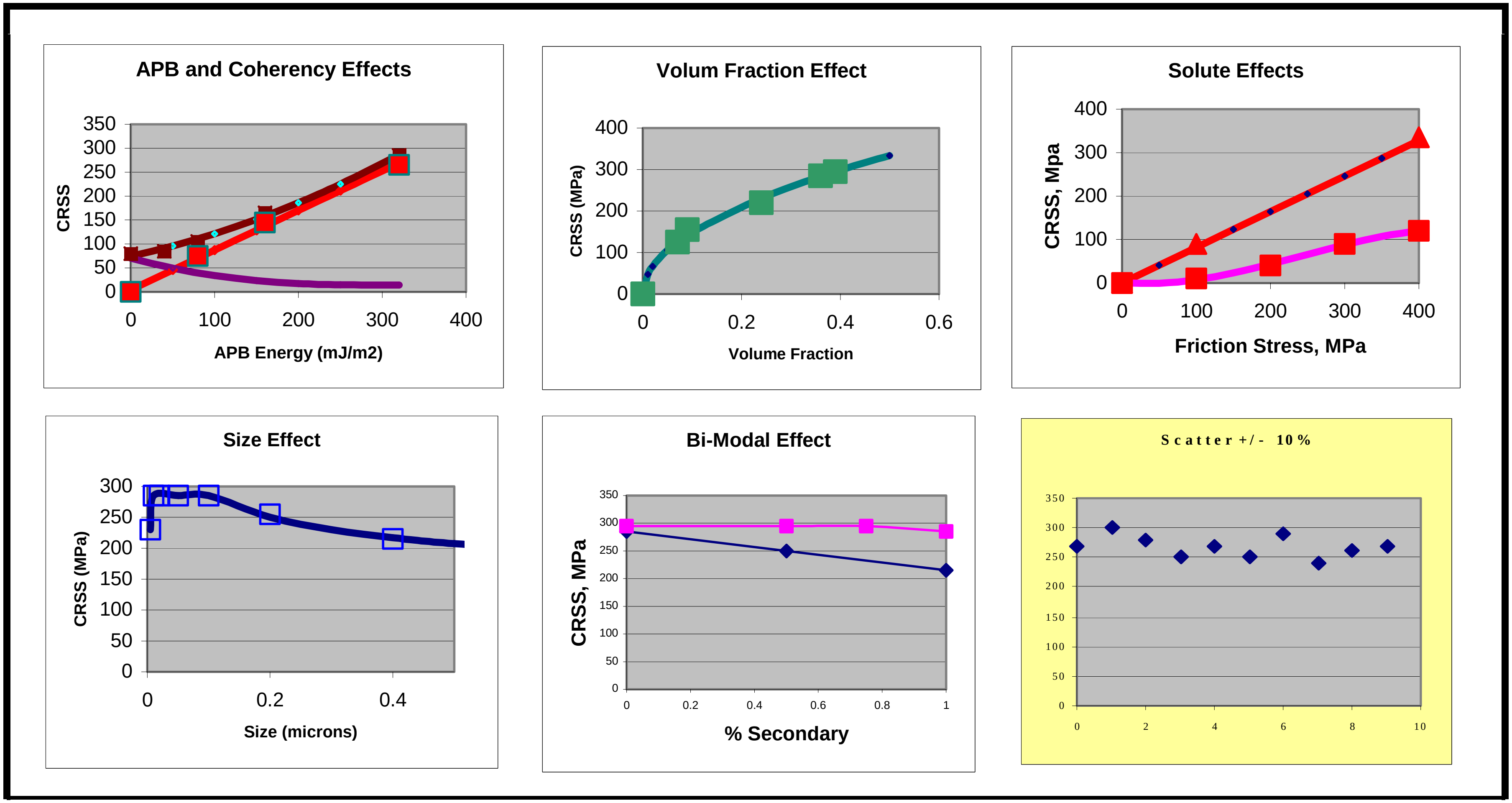
DD : Current Focus - Connectivity (“Handshakes”)



DD : Current Focus - Connectivity ("Handshakes")



DD Parametric Studies



Fits to Parametric Studies => Pollock-type Model

Pollock-type Model : (derived from DD results)

CRSS =

APB

$$Min\ \Psi \quad '' \quad (A_1\ 2\ A_2 B_{APB})\ 2$$

Coherency

Volume Fraction

$$2\ (C_1\ 4\ C_2 B_{APB}\ 2\ C_3 B_{APB}{}^2\ 4\ C_4 B_{APB}{}^3)\frac{C}{0.3} \notin \left(qV_f\right)^{0.5}$$

$$,\ \left[\ S_1\ \Psi a / V_f{}^{4\,0.5}\ 4\ 1\ 0\ \beta^{4\,S_2}\ \right]$$

Ppt Size

$$+\quad F\ ''\ \left(P_1\ 2\ P_2 \vartheta_{\nu'}\ 2\ P_3 \vartheta_{\nu'}{}^2\right),\ \left(M_1 \vartheta_{\nu}{}^{M\,2}\right)$$

Ppt Sol. Str. Matrix Sol. Str.

$$\omega_Y\ |\ (1\ 4\ f_{\nu'})''(M\ (CRSS\ )\ 2\ k_{\nu 2 \nu'} d_{\nu 2 \nu'}{}^{4\,0.5}) \in 2\ f_{\nu'} / \vartheta_{0\,\nu'}\ 2\ k_{\nu'} d_{\nu'}{}^{4\,0.5}$$

IN 100 - Spreadsheet

Data from Pollock's slides

Clement / Nembach

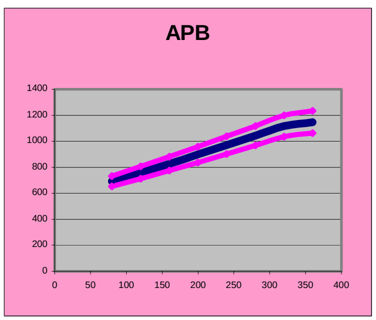
Exp. ⇨

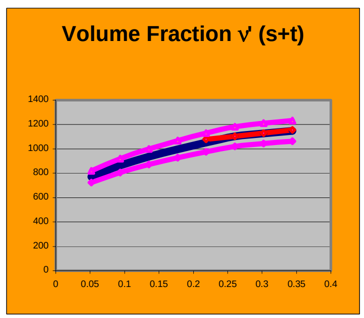
Coh %	Vf-Total	Vf-t	Size-t	Vf-s	Size-s	Vf-p	Size-p	$d_{(\gamma 2\gamma')}$	sol-g	sol-g'
0.1	0.544	0.01	0.006	0.334	0.12	0.2	1.7	3.82	100	50
0.0125				0.04175	0.015				6	6

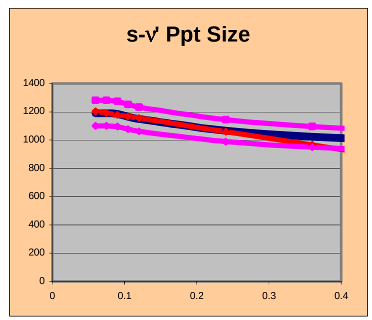
Fit Par. ⇨

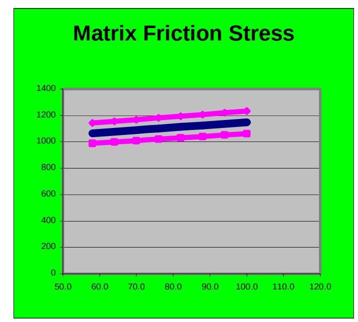
APB	M	k_γ
360	3	500
40.00		

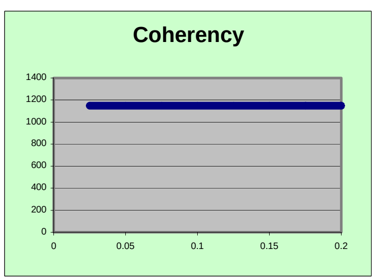
$k_{\gamma'-P\gamma}$
500





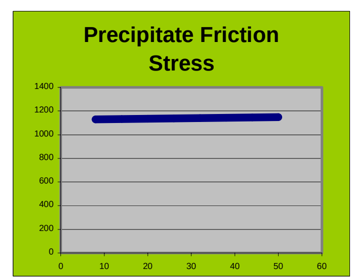






— Schirra (IN100)

YS (ksi) = 66.3 + 6.43 x ASTM Grain Size # + .89 x % Cooling g' - 114.5 x cooling g' size (in microns)



Data from Pollock on IN100 (PWA 1100 - ver.3)

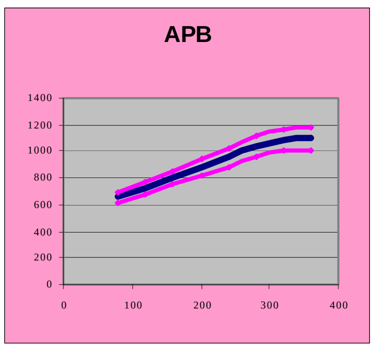
Data from Pollock's slides ← → | Clement / Nembach ↓ ↓

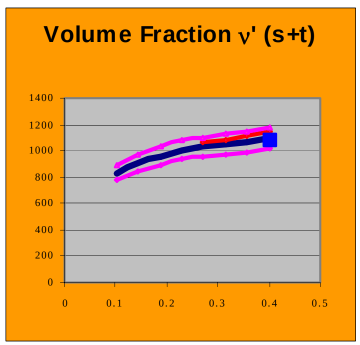
Exp. ⇨

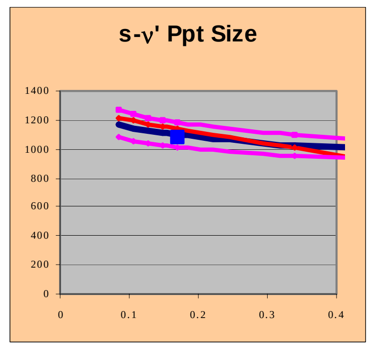
oh %	Vf-Total	Vf-t	Size-t	Vf-s	Size-s	Vf-p	Size-p	d$_{(\gamma 2\gamma')}$	sol-g	sol-g'
0.1	0.6	0.06	0.002	0.34	0.17	0.2	1.2	4.1	100	50
0.0125				0.0425	0.02125				6	6

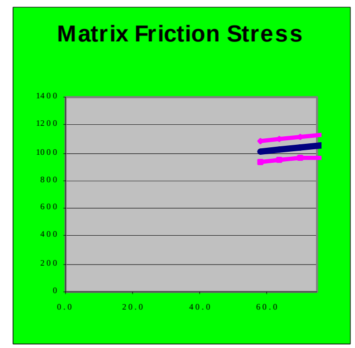
Fit Par. ⇨

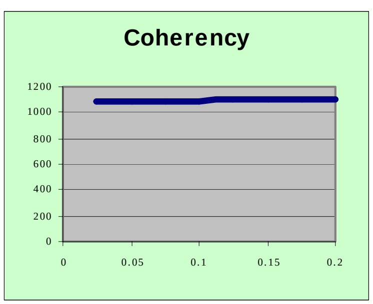
APB	M	k_γ	$k_{\gamma'\text{-Py}}$
360	3	450	450
40.00			





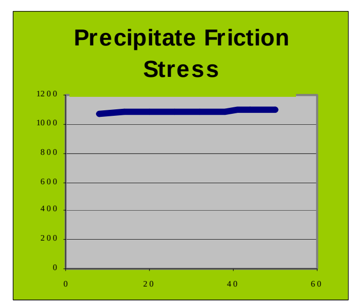






— Schirra (IN100)

YS (ksi) = 66.3 + 6.43 x ASTM Grain Size +
+ .89 x % Cooling
- 114.5 x cooling g' size (in micron



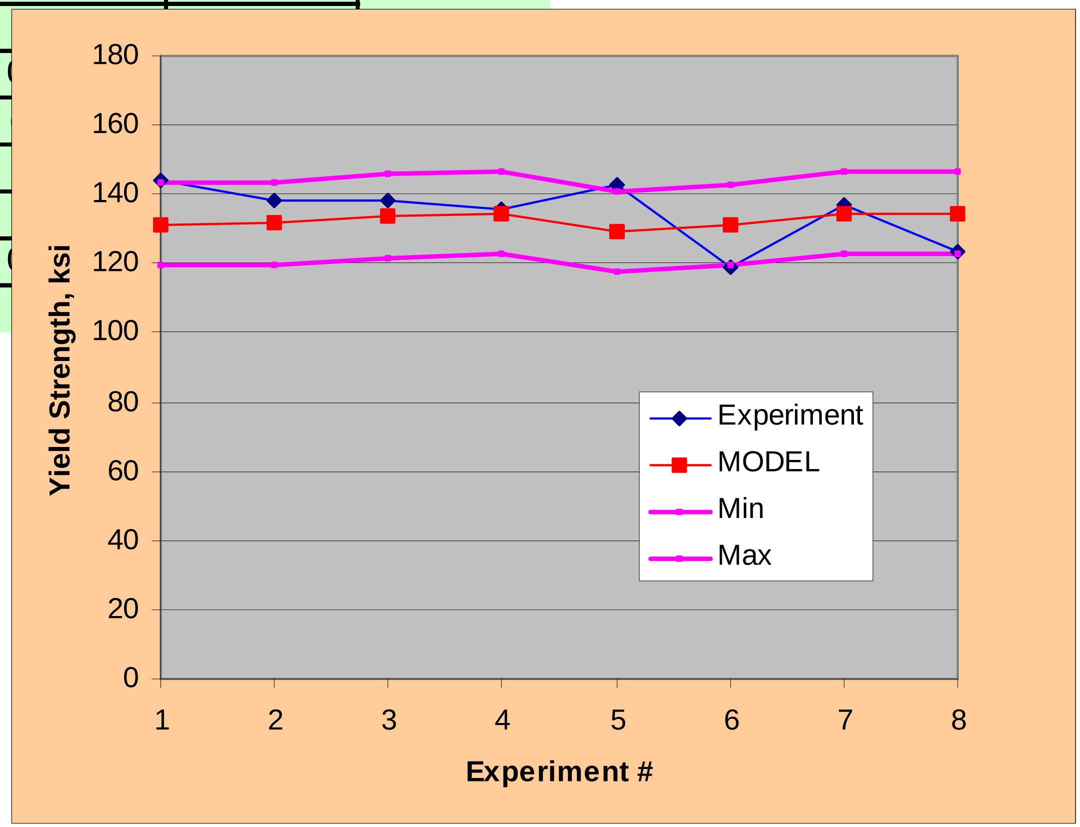
Rene 88 - 1200 F Data (from Pollock's slides)

Data from Pollock's slides

Clement / Nembach

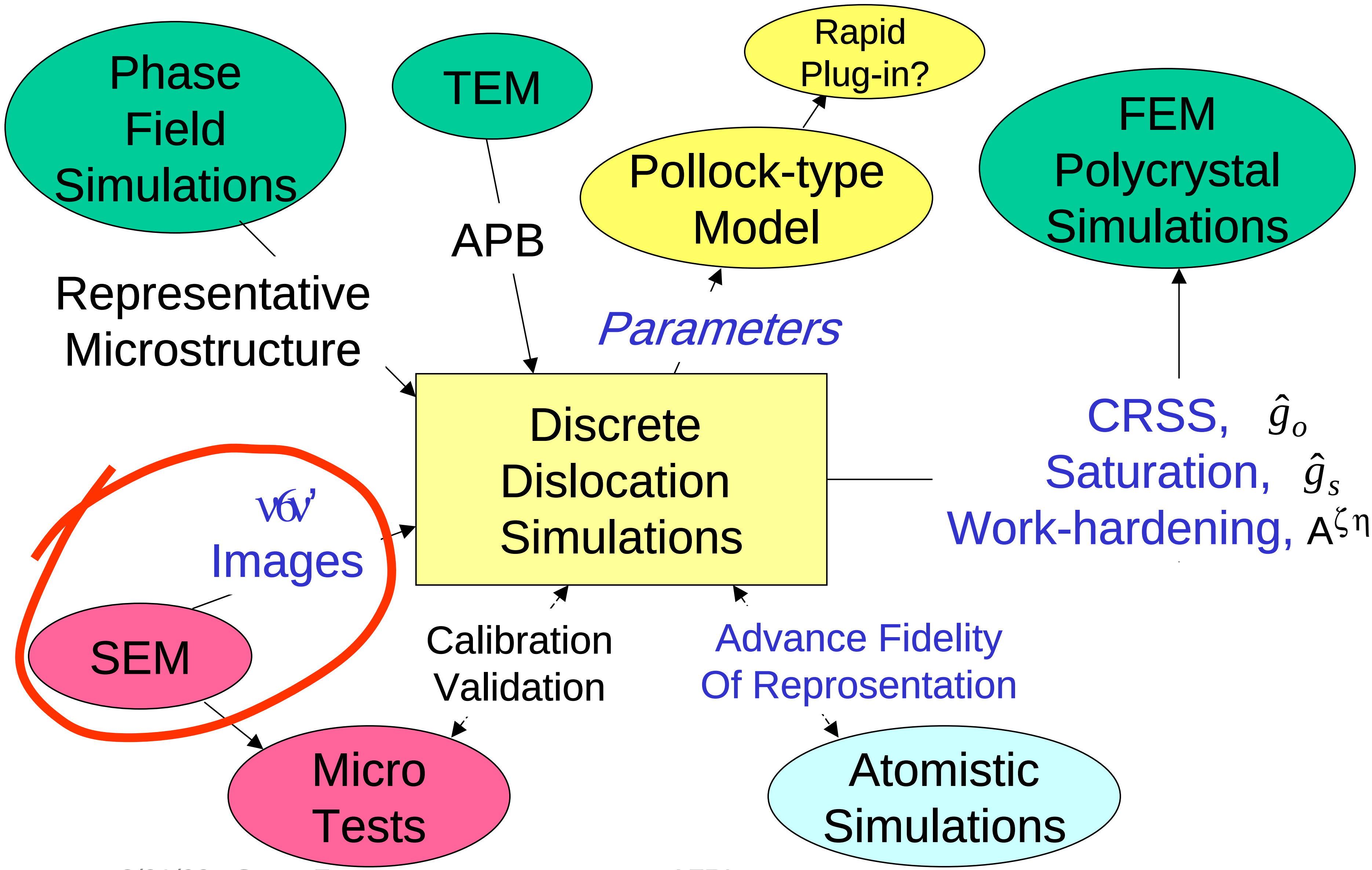
Coh %	$d_{(\gamma 2\gamma')}$	sol-g	sol-g'
0.1	28.2	33	200

Experiemental Data					
d G' (um)	G' Fraction	d G'' (um)	G'' Fractio	Yield Stres	YS (ksi)
0.1478	0.2321	0.008474	0.1822	992.88	144
0.1636	0.322	0.007317			
0.1489	0.32487	0.0393			
0.1669	0.3346	0.0153			
0.2738	0.1322	0.0083			
0.3865	0.2708	0.008			
0.2477	0.2416	0.017			
0.39	0.2771	0.0318			



APB	M	k_y
240	3	500

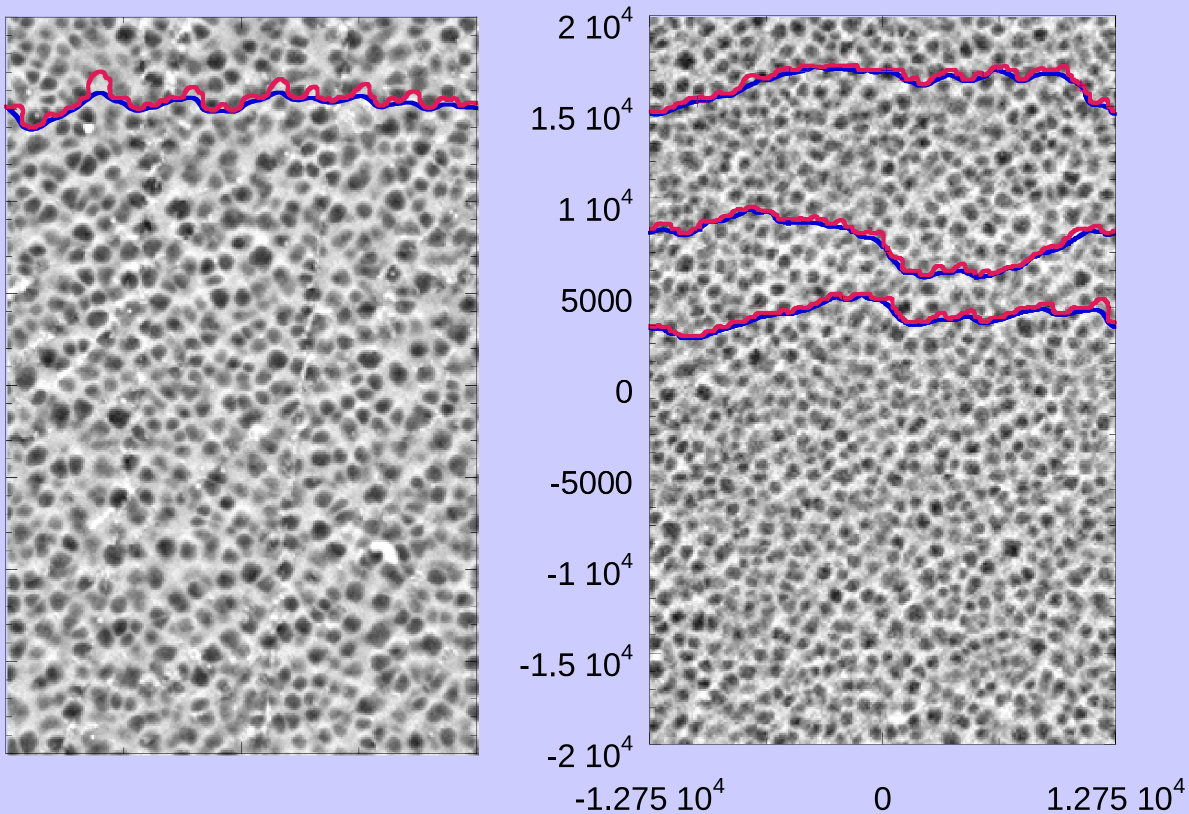
DD : Current Focus - Connectivity (“Handshakes”)



SEM Image -> CRSS

Bore **Rim** **Web**

ϑ= 275 MPa **ϑ= 275 MPa** **ϑ=265 MPa**



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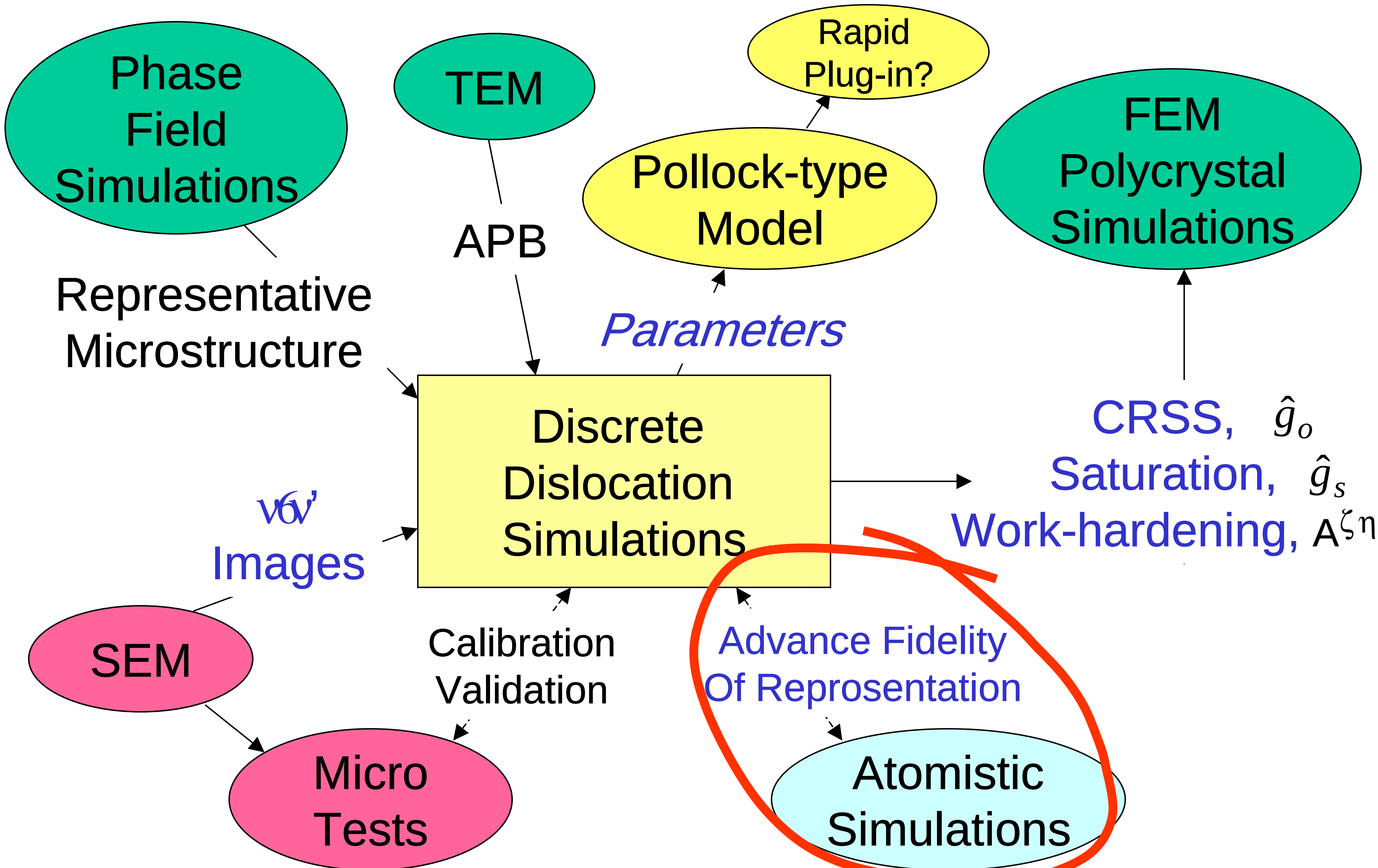
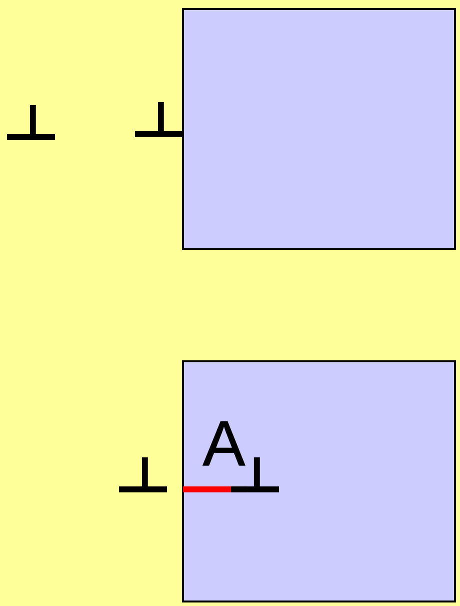


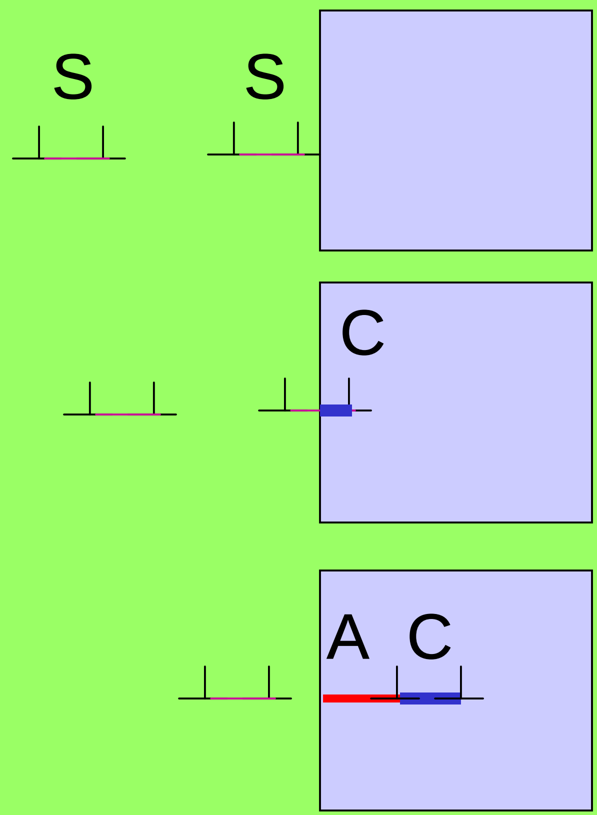
Atomistic Simulations -> Refinements of DD

DD Neglects Core Effects



APB Energy
Critical Parameter

Atomistics Include Core Effects



CSF, Core Effects Important ?
(Cross-slip within ν')

Atomistics Simulation Validation Results

- EAM Potential with APB=140, CSF=120, SF(Ni)=60

- FLAT INTERFACE :

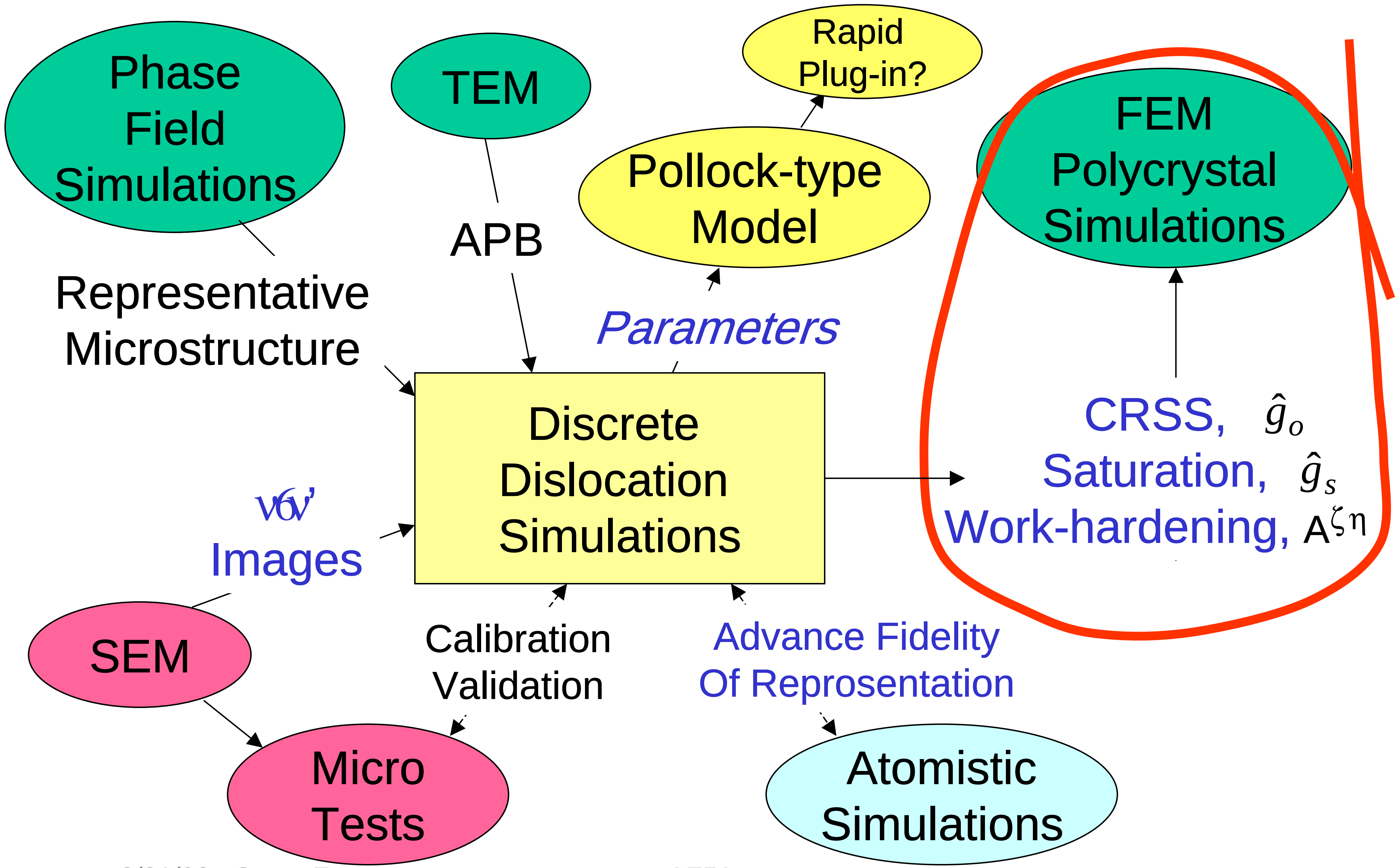
<u>Atomistics</u>

- Stress for first partial to enter : (CSF-SF) / b
- Stress for second partial to enter : (APB) / b
- No diffuse core effect

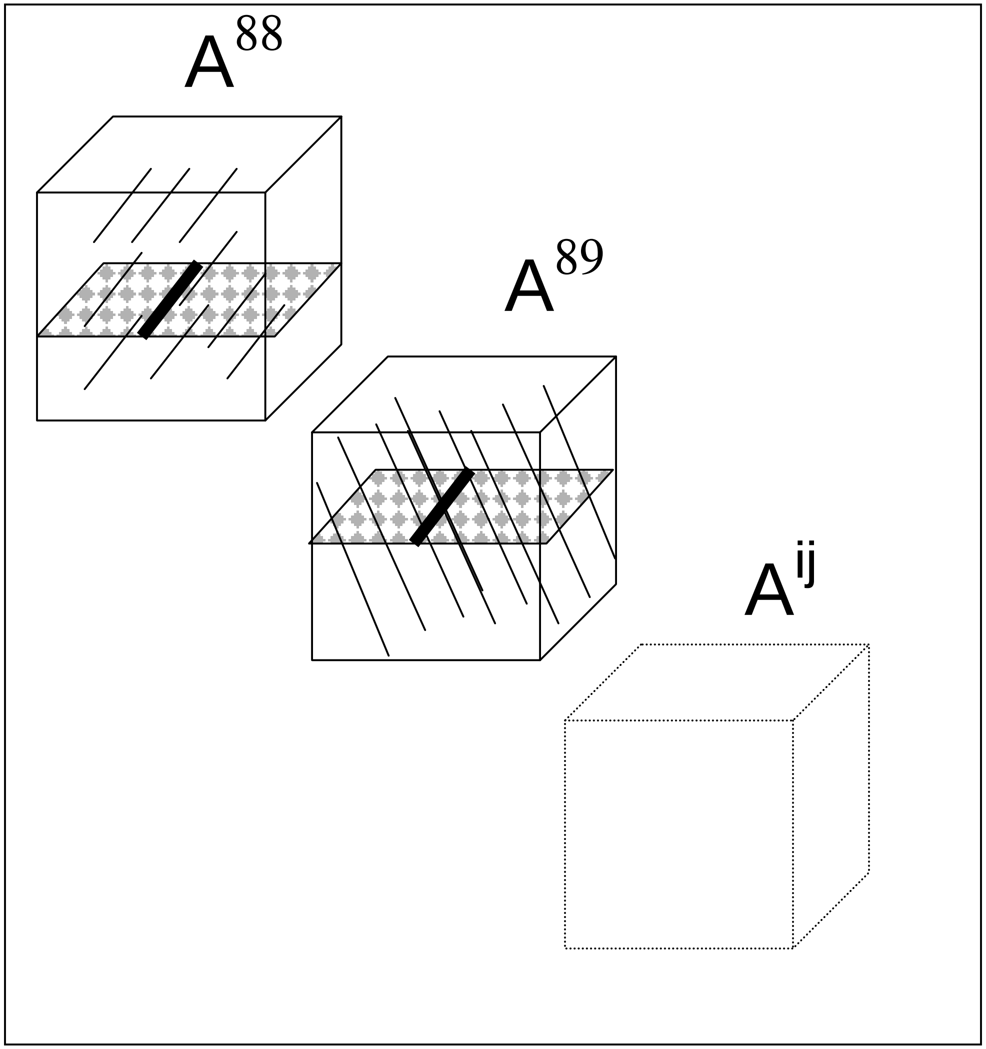
<u>DD</u> Max Stress = Stress for 1^{st} Disln entry = (APB)/b

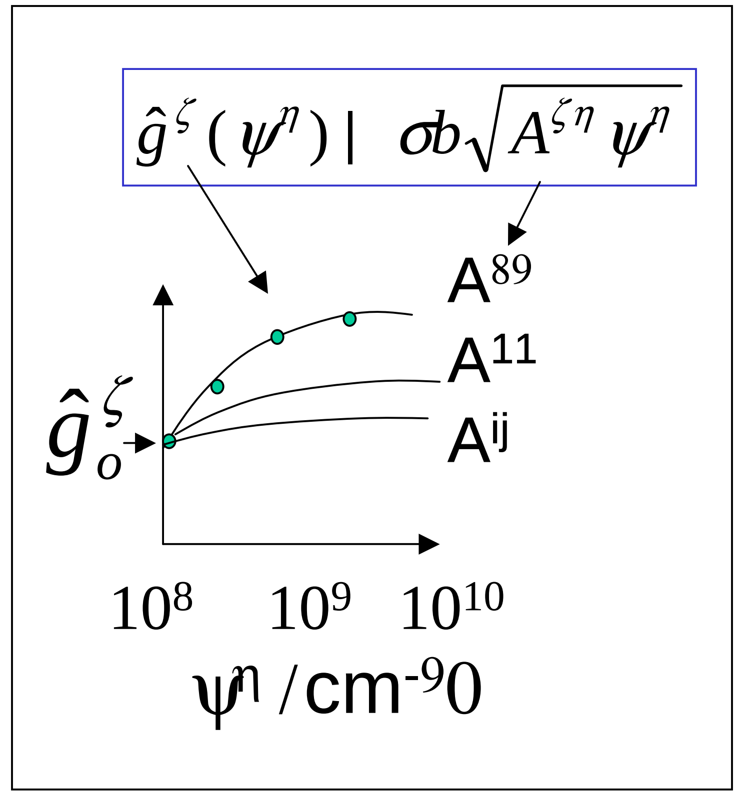
=> APB Energy Sufficient , if APB (CSF-SF)

DD : Current Focus - Connectivity ("Handshakes")



DD -> FEM Handoffs





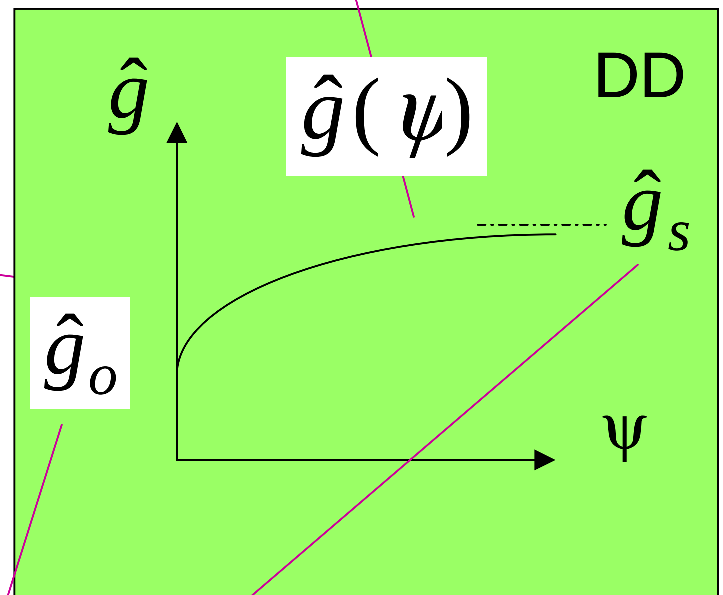
DD -> FEM Handoffs

- γ Forest Obstacle Model (*Franciosi, 1985*)

$$\hat{g}^{\zeta} \mid \hat{g}_o \, 2 \, \sigma b \sqrt{\sum_{\eta} A^{\zeta\eta} \psi^{\eta}}$$

Strengthening interaction coefficients

Initial Hardness = CRSS



GND *Stat. Stored*

$$\dot{\hat{g}} \mid \frac{\xi^2 \sigma^2 \mathbf{b}}{2(\hat{\mathbf{g}} \, 4 \, \hat{\mathbf{g}}_o)} \mathbf{k}_o \sum_{\zeta} \dot{\zeta}^{\zeta} \left| \dot{\psi}^{\zeta} \right| 2 \chi \sum_{\zeta} \left| \dot{\psi}^{\zeta} \right|$$

$$\chi \mid \chi_o \left(\frac{\hat{\mathbf{g}}_s \, 4 \, \hat{\mathbf{g}}}{\hat{\mathbf{g}}_s \, 4 \, \hat{\mathbf{g}}_o} \right)$$

OUTLINE

Microstructure Effects Within Grains (ν2ν')

Using DD SIMULATIONS (S.Rao, T.A.Parthasarathy, D.M.Dimiduk, P.M.Hazzledine)

- PROGRESS : Established a Working Model / Methodology
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Using FEM (Y-S Choi, T.A.Parthasarathy, D.M.Dimiduk)

- Unit Cell Model : Identified Key Issues - Refinements

Grain-Grain Interaction

- Polycrystal Model : Using DD results

Grain-Defect Interaction

FEM : Unit Cell Model (Single Grain)

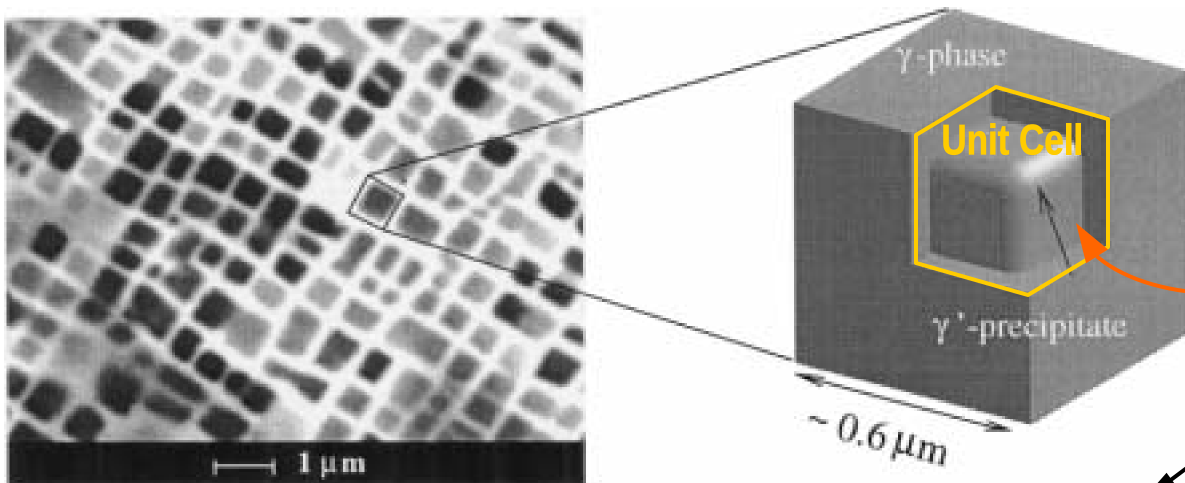
- Evaluated Unit Cell Approach using A-B Formalism

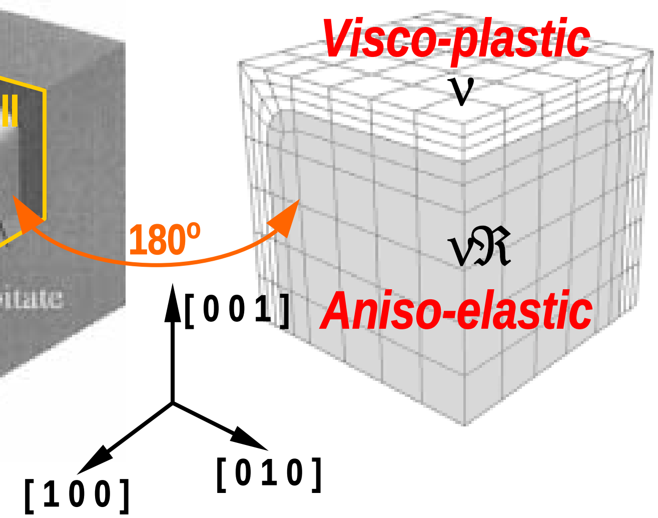
  - Yield Point -> determined by geometrical constraint (different mechanism than DD)

  - W-H beyond Yield -> strain-gradient term dominant

- Refinement : Relaxation of Elastic ν' (using DD results)

FE Simulation of (ν+ν') : Unit Cell Approach





From Busso et al., J. Mech. Phy. Sol., 48(2000), pp 2333~2361.

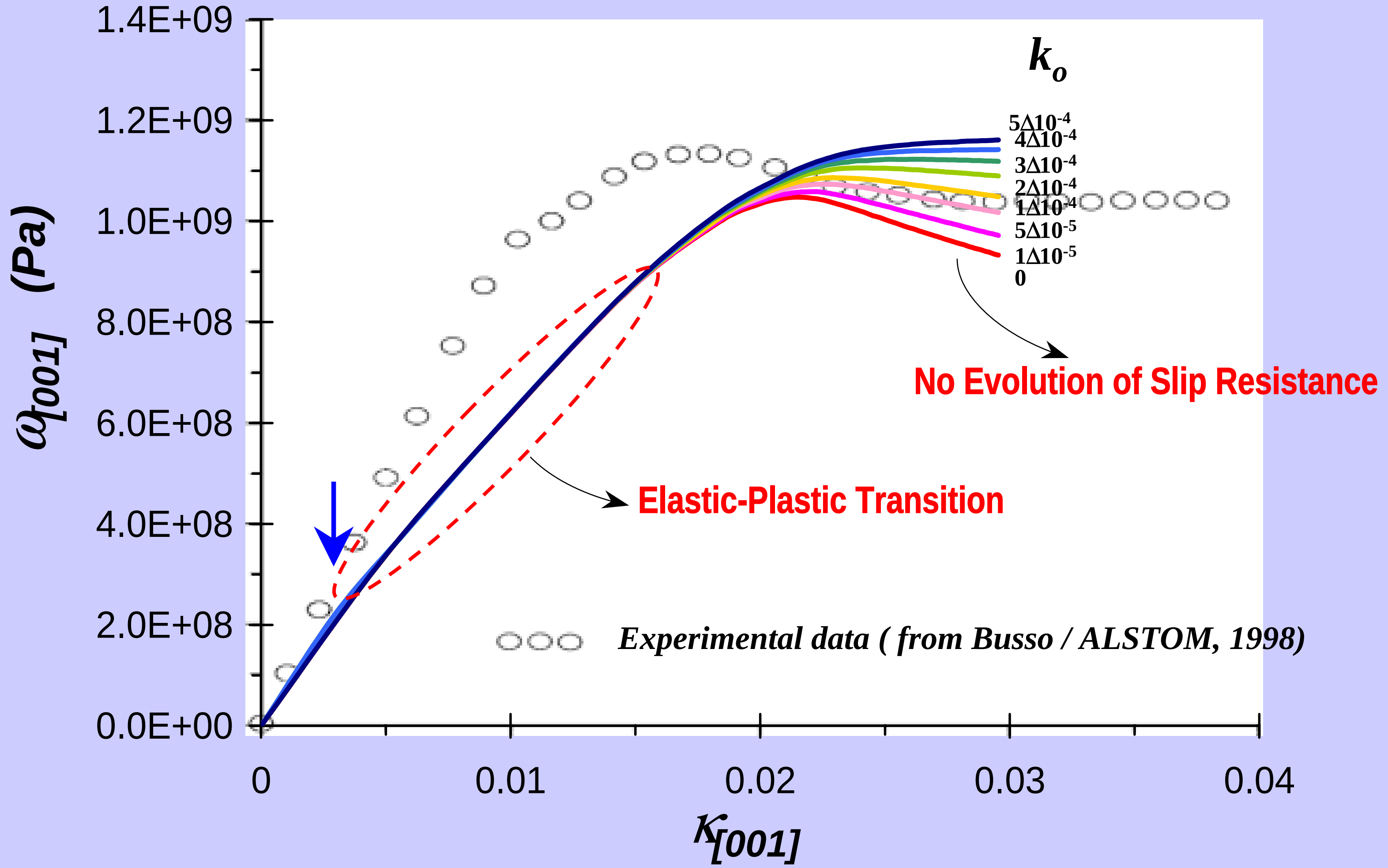
$$\dot{\gamma}^{\zeta} = \dot{\gamma}_o \,\mathrm{sgn}(\tau^{\zeta}) \left| \frac{\tau^{\zeta}}{\hat{g}^{\zeta}} \right|^{1/m}$$

with

$$\dot{\hat{g}} = \frac{\xi^2 \sigma^2 b}{2(\hat{g} - \hat{g}_o)} k_o \sum_{\zeta} \varsigma^{\zeta} \left| \dot{\gamma}^{\zeta} \right|$$

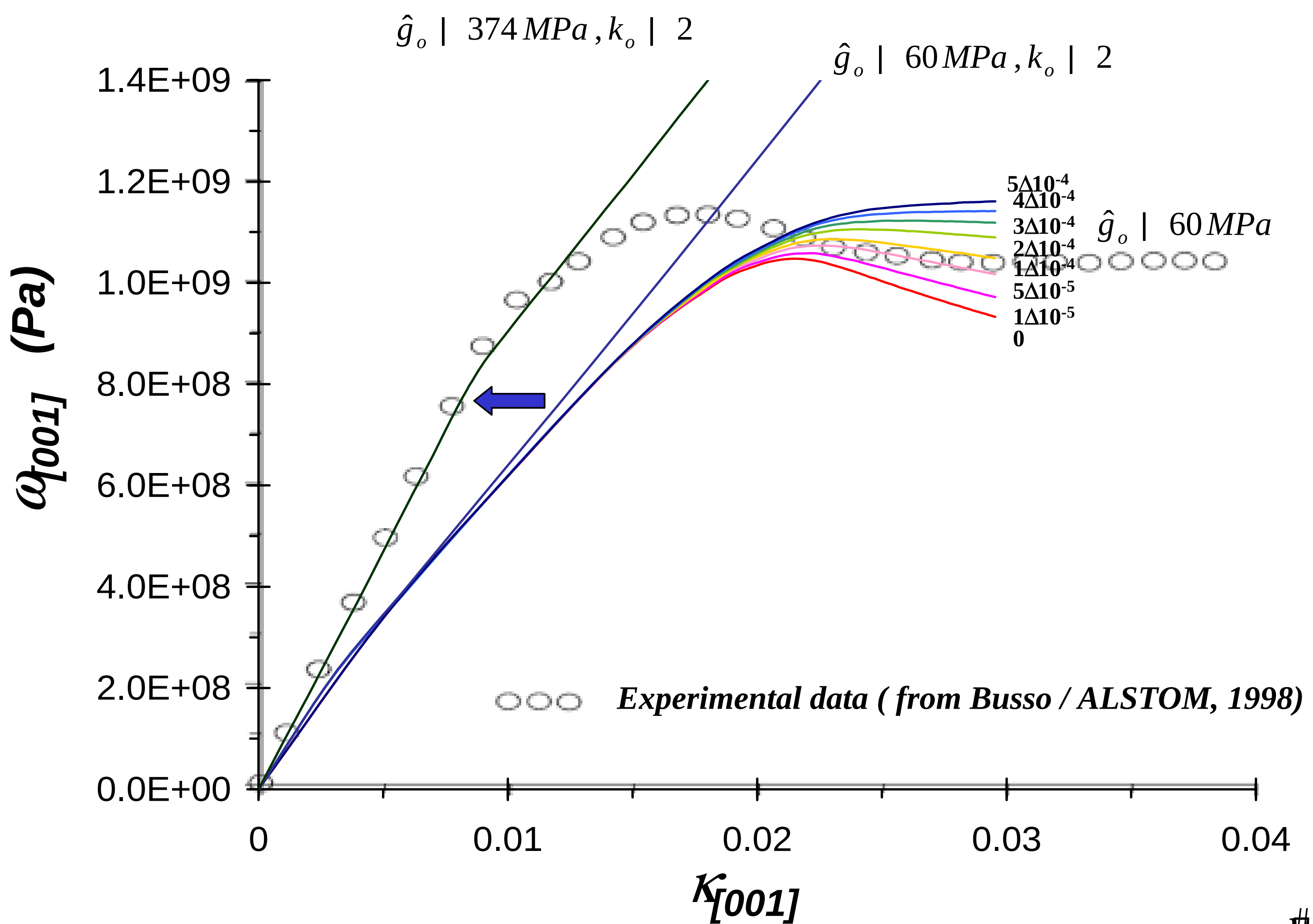
Only ς^{ζ} (GND) contribution to slip resistance.

Effect of Strain-Gradient Parameter: k_o



$\hat{g}_o \,|\, 60\,MPa,\ m \,|\, 0.03,\ \dot{\gamma}_o \,|\, 0.001$

Effect of $\hat{g}_o$

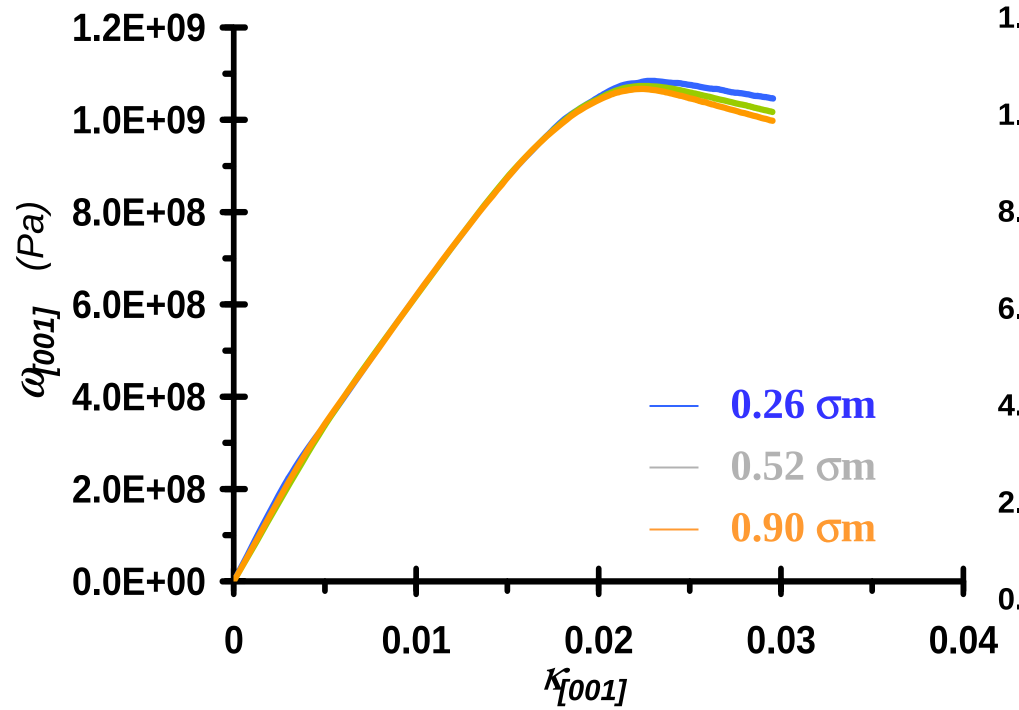


$\not{v}_o$ | 0.001

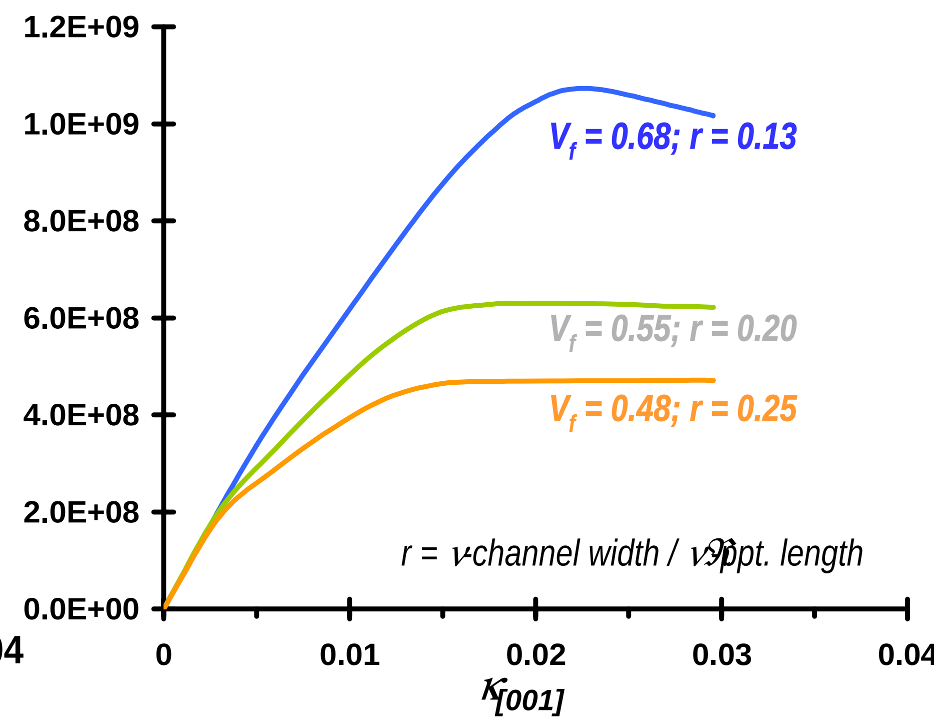
$\hat{g}_{t2\div t}$ | $\hat{g}_{t2\div t}\div t\ 2\ \hat{g}_t$

Length Scale Effects : ν' Size, V_f

- Constant ν' ppt. V_f = 68%
- Change ν' size (ν-channel width)



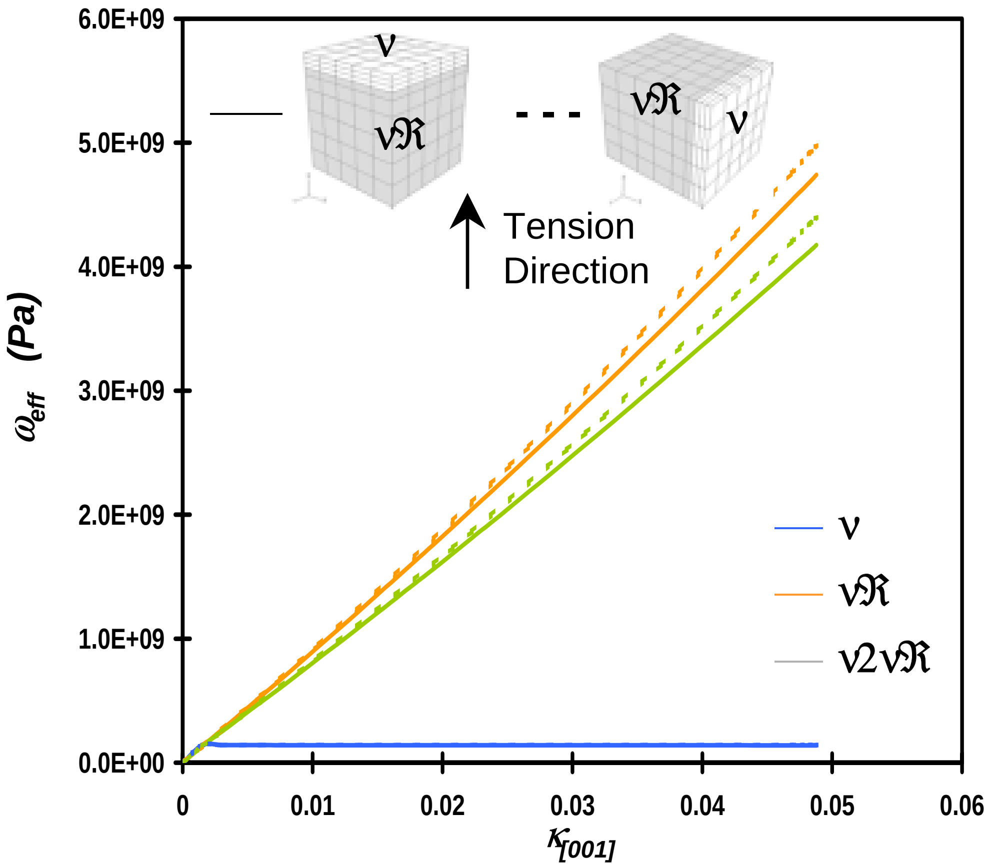
- Constant ν' size = 0.52 σm
- Change ν' V_f (ν-channel width)

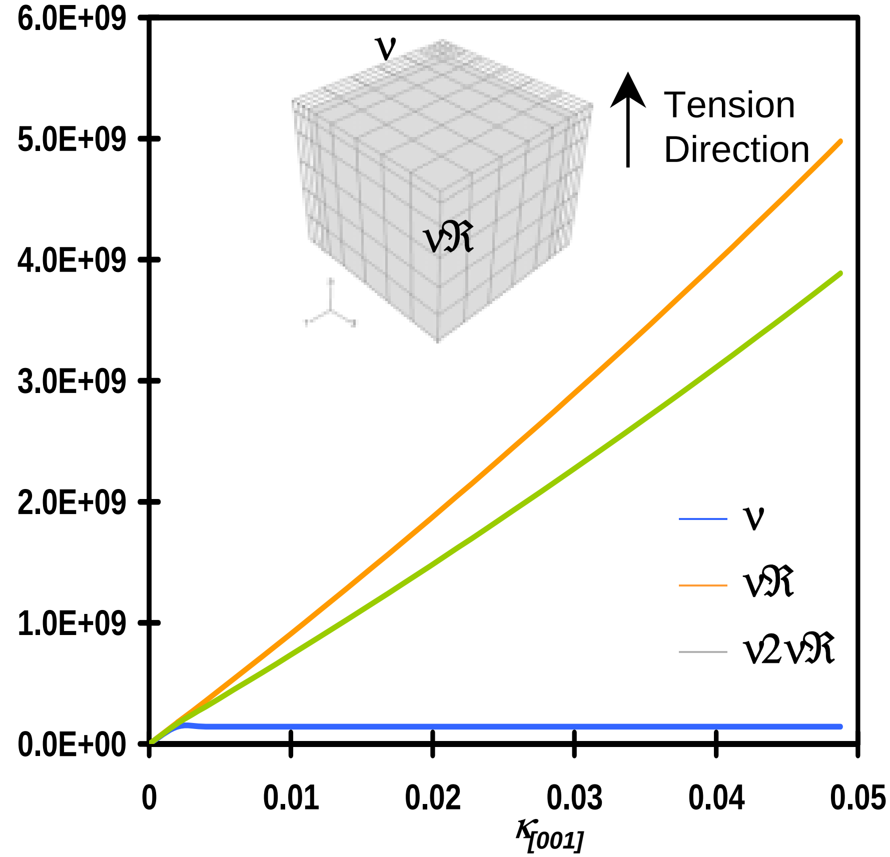


- $\hat{g}_o \mid 60\,MPa, m \mid 0.03, \dot{\varepsilon}_o \mid 0.001, k_o \mid 5\Delta10^{45}$

Effect of ν/ν𝔑3D Geometry

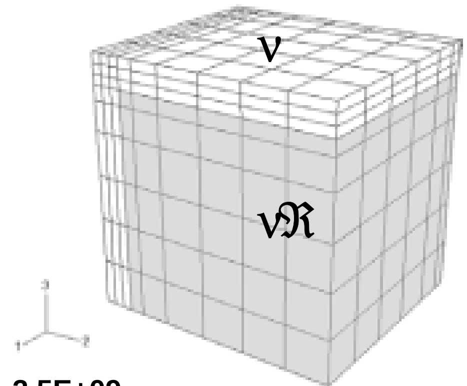
- **Elastic ν𝔑2 Elasto-viscoplastic ν**
- $\hat{g}_o \mid 60MPa, m \mid 0.03, \dot{\gamma}_o \mid 0.001, k_o \mid 0$ for Viscoplasticity



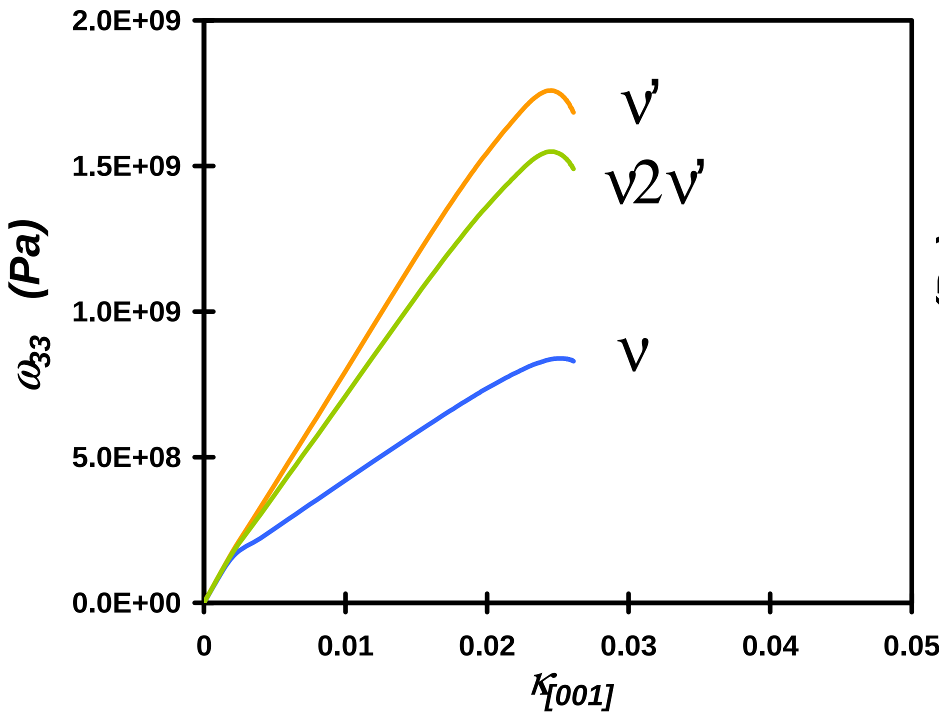


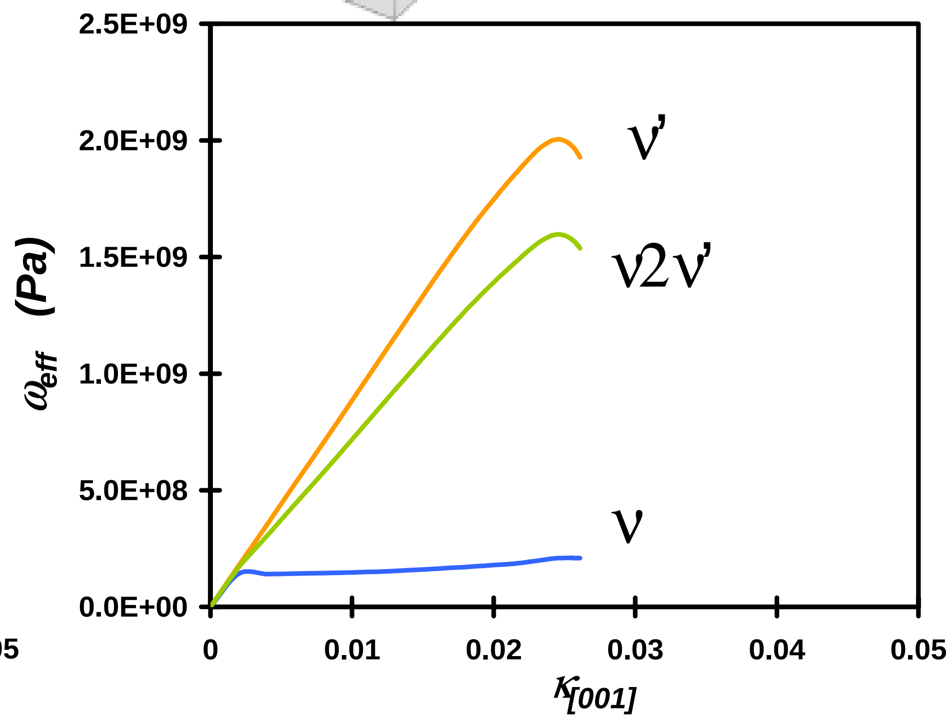
Effect of ν/νℜ3D Geometry

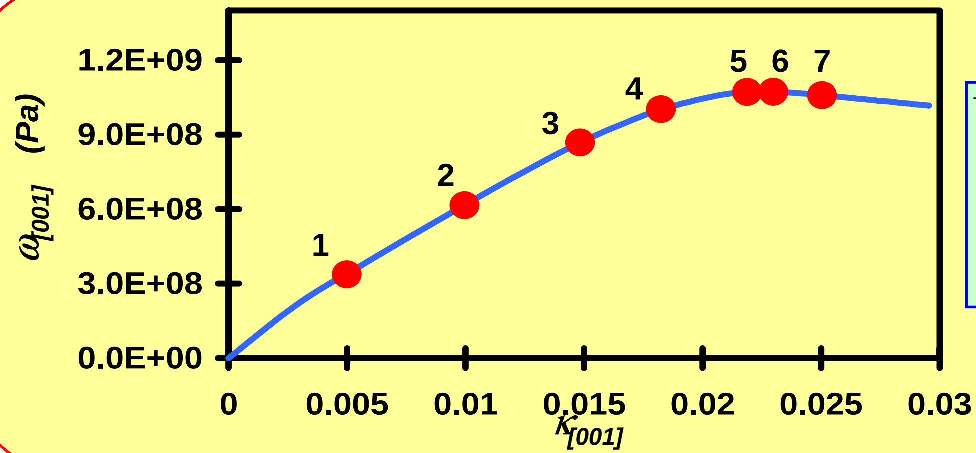
- **Elastic νℜ2 Elasto-viscoplastic ν**
- $\hat{g}_o \mid 60MPa, m \mid 0.03, \dot{\gamma}_o \mid 0.001,$
  $k_o \mid 0 \;\; for \;\; Viscoplasticity$



Tension
Direction



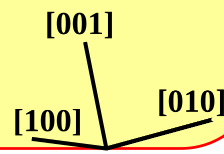


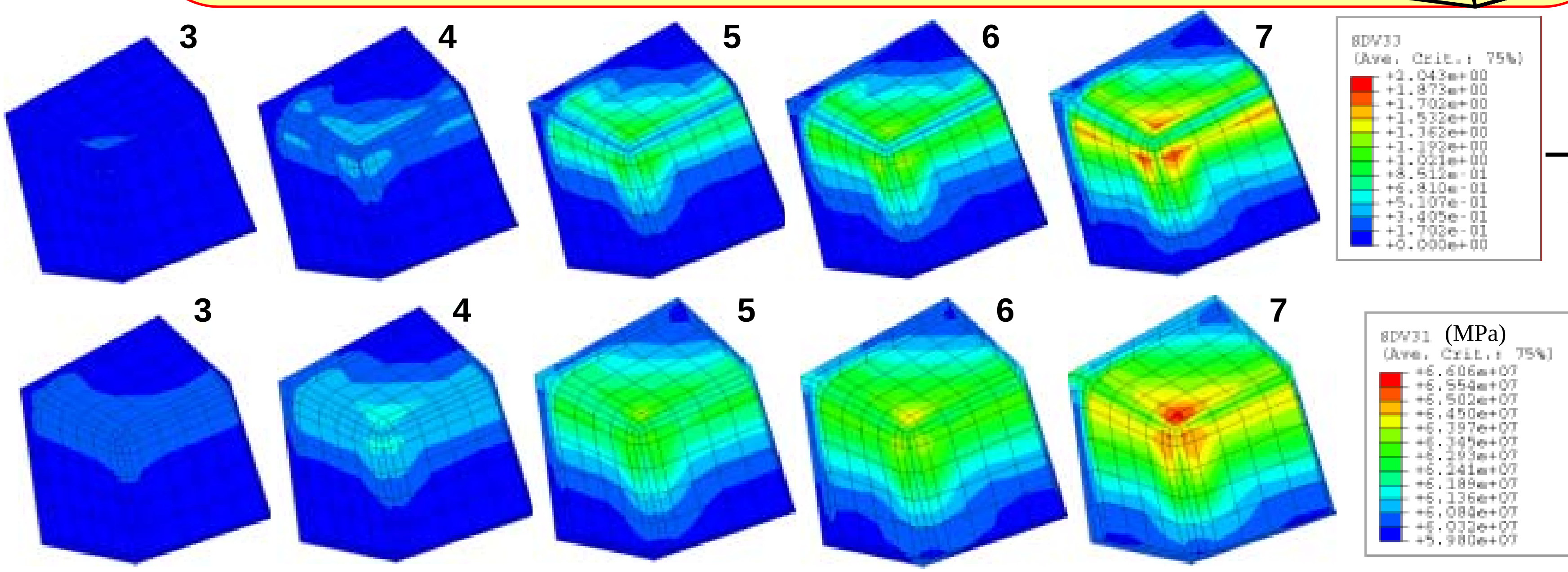


V_f | 68%, νℜsize | 0.52 σm

$\hat{g}_o$ | 60 MPa, m | 0.03

$\dot{\gamma}_o$ | 0.001, k_o | 5Δ10^{45}





ν^{ζ}

$\hat{g}$

- The onset of softening accompanied by the massive shears localized along the edges and the corners in the ν/νℜ interfaces
  - ♥ Break down of geometric (kinematic) constraints
  - ♥ Need to compare with experimental observations at this particular T-range

FEM : Unit Cell Model (Single Grain)

- Evaluated Unit Cell Approach using A-B Formalism
  - Yield Point -> determined by geometrical constraint
    - captures V_f Effect
  - W-H beyond Yield -> strain-gradient term dominant
    - captures size effect during work-hardening
- Refinement : Allow Plasticity in γ' (using DD results)
  - DD captures APB cutting,
  - FEM captures Geometrical Constraint effect and Work Hardening

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- Unit Cell Model : Identified Key Issues - Refinements

Grain-Grain Interaction

- Polycrystal Model : Using DD results

Grain-Defect Interaction

FEM : Polycrystal Model

- FY 2003 Goal : Combine DD with FEM to Build 1st gen. (ν2ν') Polycrystal model
  - Wigner-Seitz Cell (Beaudoin) - (144 grains, 12 el/gr)
  - Use DD results for g_o and A_{ij}
  - A-B model for Strain-gradient Terms

- Beyond FY2003
  - Build/Borrow ν' const. Law to Model IN100 type alloy
  - Real Image 3D Polycrystal Models
    - Adaptive Meshing of Realistic Microstructures

Building Bridges : Inputs for Pollock-type Model

$$\omega_y(C_i, T, \kappa, \dot{\kappa}, \ldots) =$$

Needs Development Within Atomistics

$$f_\nu \left(\frac{T_o}{T}\right)\left(\sum_i \frac{dc}{\sqrt{dC_i}}\sqrt{C_i}\right) + M f_t \left(\frac{\mathrm{B}_{APB}}{b}\right)$$

Obtain by Dislocation Kinetics Simulation

$+$

$$M \frac{4}{\phi^{1.5}} \left(\frac{T_L}{bd_s}\right) \sqrt{f(1-f_p)} \sqrt{\left(\frac{\phi d_s \nu}{2T_L}\right) - 1}$$ **strong coupling**

$$M \left(\frac{\mathrm{B}}{2b}\right)^{1.5} \sqrt{\frac{2bd_s f(1-f_p)}{T_L}} \left(\frac{4}{\phi^{1.5}} - \frac{\mathrm{B} f(1-f_p)}{2b}\right)$$ **weak coupling**

Obtain by FEM Simulation of Grain Distribution Effects

$$+ (1-f_p)k_y^{\nu} \frac{1}{\sqrt{d_\nu}} + f_p\left(\omega(T)_{Ni_3Al} + \sum_i \left(\frac{dc}{dC_i}\right) C_i\right) + f_p k_y^{\nu\Re} \frac{1}{\sqrt{d_{\nu\Re}}}$$

Building Bridges ....

TO

- Inputs for Pollock-type Model 3-6 mo.
- Fatigue Models (McDowell,..) 1-2 yrs

FROM

- √ Constitutive Laws (Parks, Cuitino/Ortiz, ...) 3-6 mo.
- 3D Voronoi Meshing (Parks, Gosh, ..) 3-6 mo.