Modeling Materials Properties: A Selective & Brief Introduction (Especially for Metals)

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2015 UCSB Workshop on Collection and Analysis of Big Data in 3D Materials Science

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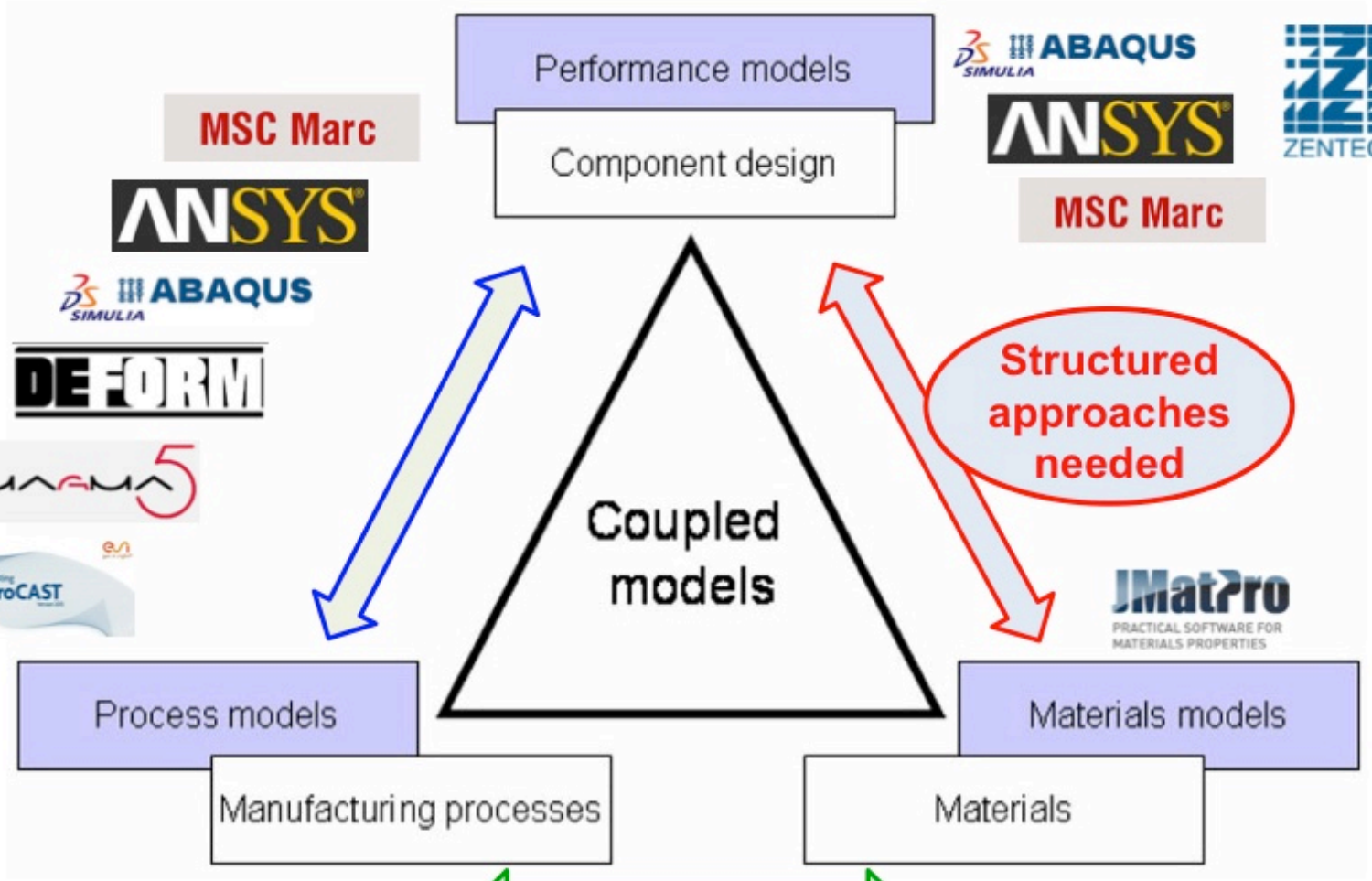
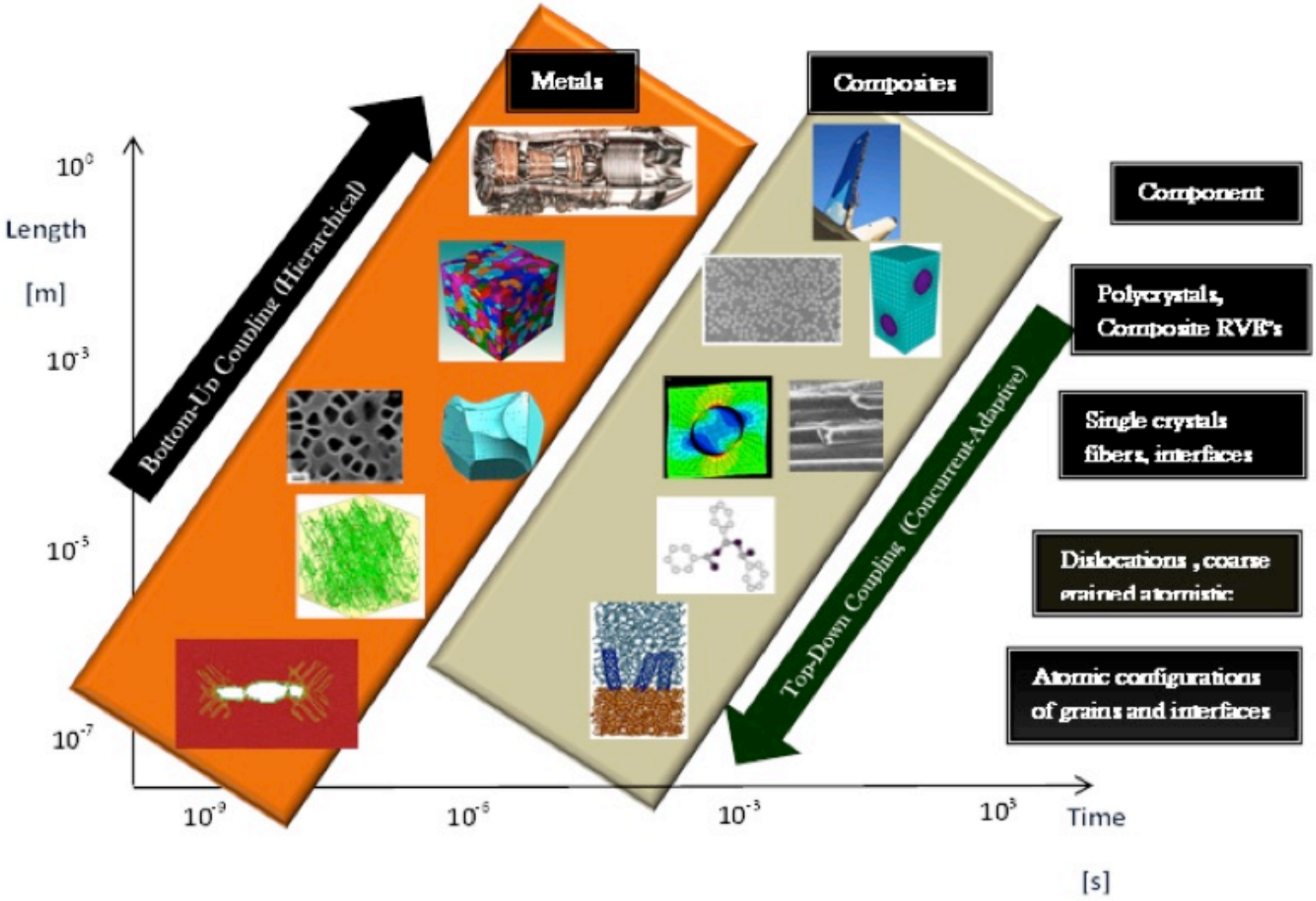
Integrated Design-Manufacturing-Materials



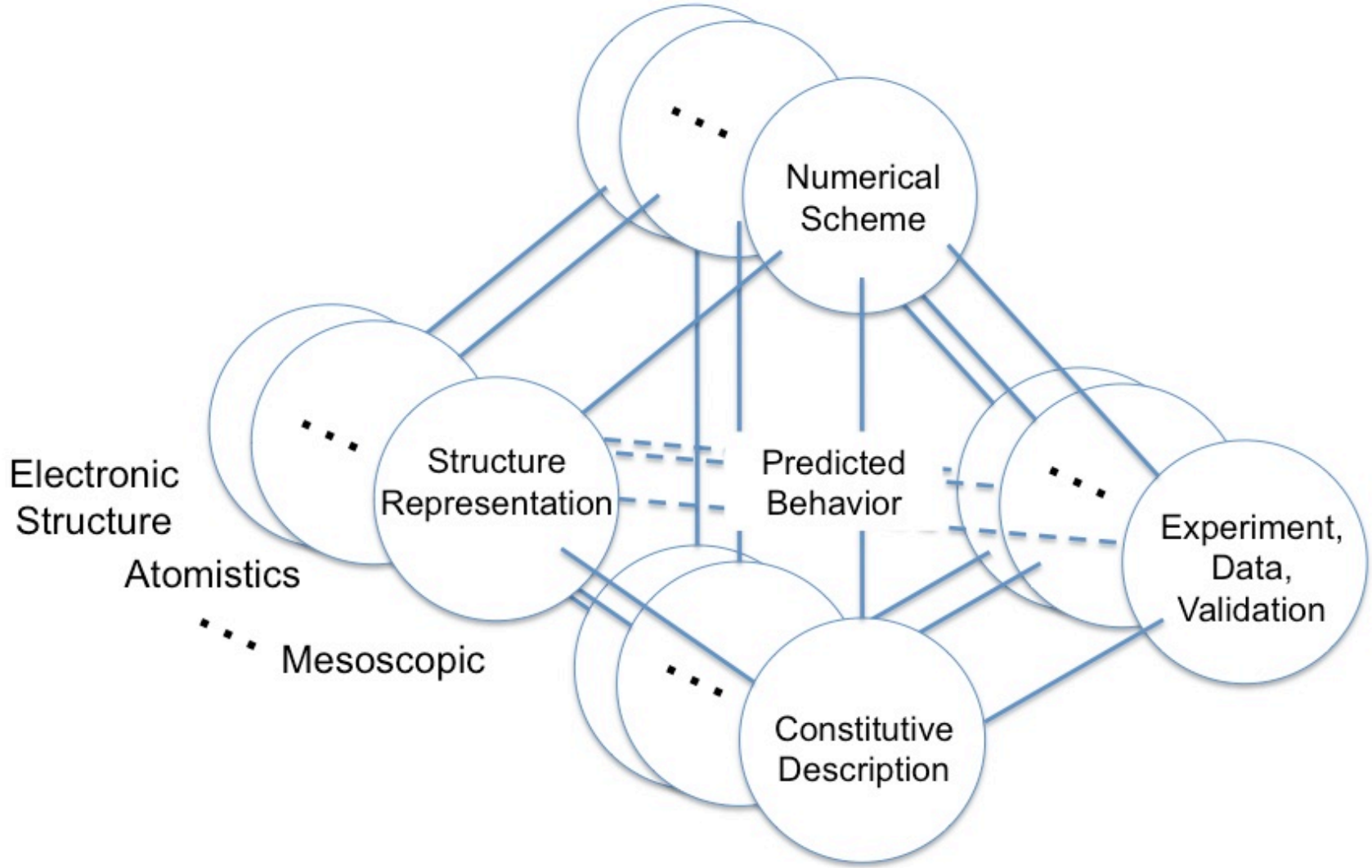
Our Reductionist Hypothesis… Scale Separation



Scale separation hypothesis is only ever probabilistically true…

adapted from S. Ghosh, et al. (2013)

Domains of Freedom for Materials Simulations



Materials data structures must be set up for models in all cases

Dimiduk, 2011

VASP & Other DFT

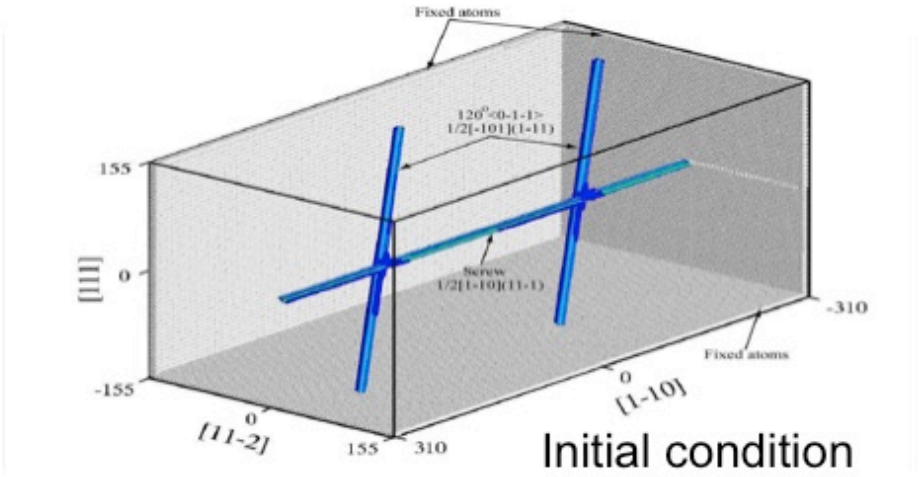
- Only “proper” methods for chemistry effects
- Lattice energies, elastic properties
- Point defect & fault energies
- Dislocation cores, “ideal” Peierls stress
- Not really for plasticity, or even many mechanisms yet…
- Some work on strain-induced transformations
  - See D. Trinkle, et al.; R. James, et al. (DeGraef MURI)
- Excellent for equilibrium properties (enthalpy of formation/ configuration, lattice parameter, elastic properties, etc.)
- Selectively used for MD
  - Chris Woodward’s viscosity of liquid superalloys; interface/fault energies, etc.
  - Others

LAMMPS —The Workhorse for MD

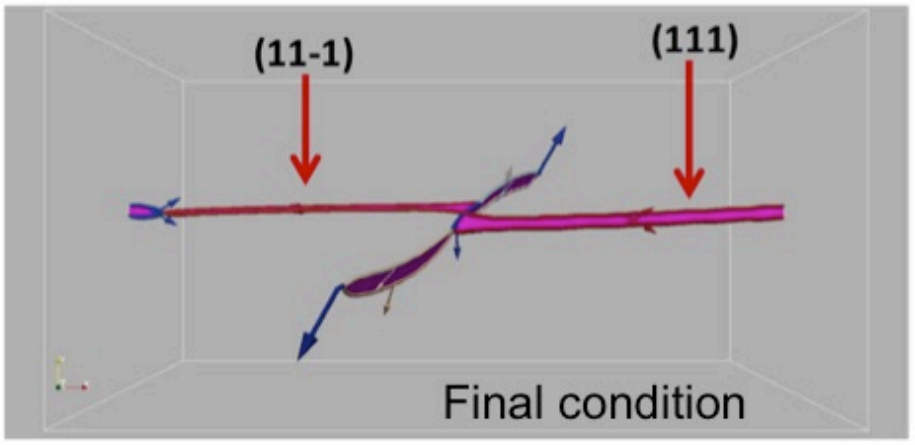
- Represent atomic interactions in a “homogenized electrons” model
- Often, not always, “spherically-symmetric atoms” (angular in MEAM)
- Less than 3rd NN interactions, maybe angular interactions
- Lattice models, with atomic positions for surface, point & line defects
- Molecular Statics —equilibrium
  - Be careful about initial conditions & boundary conditions
- Molecular Dynamics —kinetics
  - Time scales are a major barrier (~psec, maybe nsec)
  - Surprisingly effective scaling methods & stochastic models are being used to accelerate MD
- Highly scalable to largest computing platforms ☺
- Answers depend upon choice of inter-atomic potentials… ☹
- NIST project for inter-atomic potential library project

Selected LAMMPS Results

Mildly-Repulsive 120° Dislocation
Intersection Cross Slip

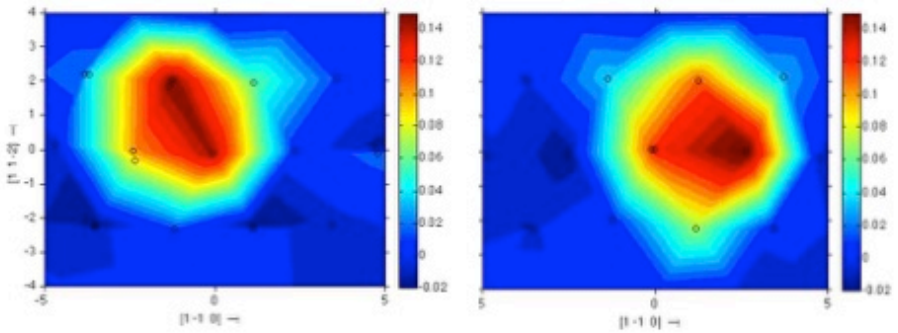


Initial condition



Final condition

$Fe_{36.67}Ti_{30}Co_{16.67}Ni_{16.67}$
BCC Alloy, Nye Tensor Maps



~32 x 10^6 atoms

½[1-10] screw dislocation core in a model FCC $Ni_{36.67}Co_{30}Fe_{16.67}Ti_{16.67}$

Initial and final configurations compared via analysis of discrete atomic positions

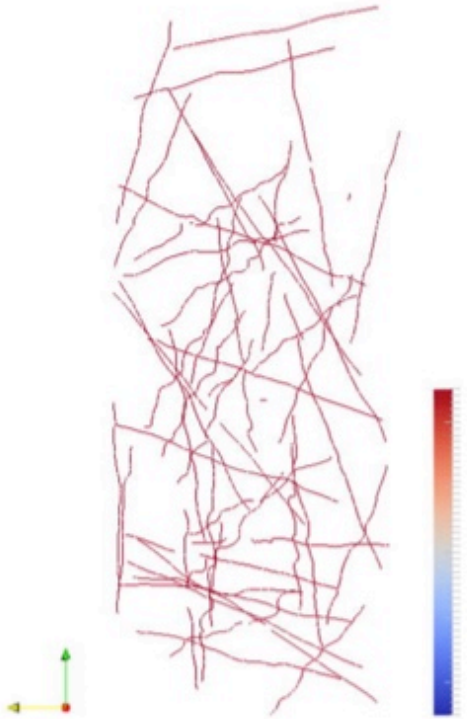
after S.I. Rao, et al. (2009 – present)

2d & 3d Discrete Dislocation Dynamics

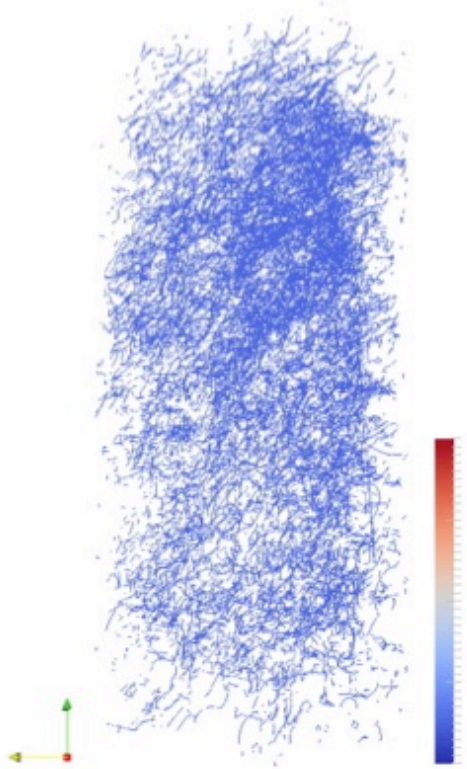
- Dislocations represented by nodes (ParaDiS) & stress-dependent velocity law (constitutive model); solve all nodal interactions
- Sometimes as lines (N. Ghoniem), or lines on a grid (B. Devincré)
- Other: M-Carmen Miguel, et al., 2d avalanches; many others
- Bulatov, Devincre, Ghoniem, Rao, El-Awady et al., 3d ParaDiS, other codes (several open source, "non-commercial")
- Method is only for experts… be careful with what is claimed…
- Major victory ☺: First & best understanding of size effects in microcrystals!
- Some weaknesses:
  - Big computing needed (the very biggest still not enough…)
    - "years" of computational time for a 20 x 20 x 50 micrometer cells…
  - Time scaling (our 50/sec is a slow strain rate, usually ~10^4/sec)
    - Stochastic cross-slip, no climb yet (emerging)
  - Simulation geometries, boundary conditions very limited so far…
  - Analysis tools *ad hoc* and inadequately developed…

3d-DD Example Results

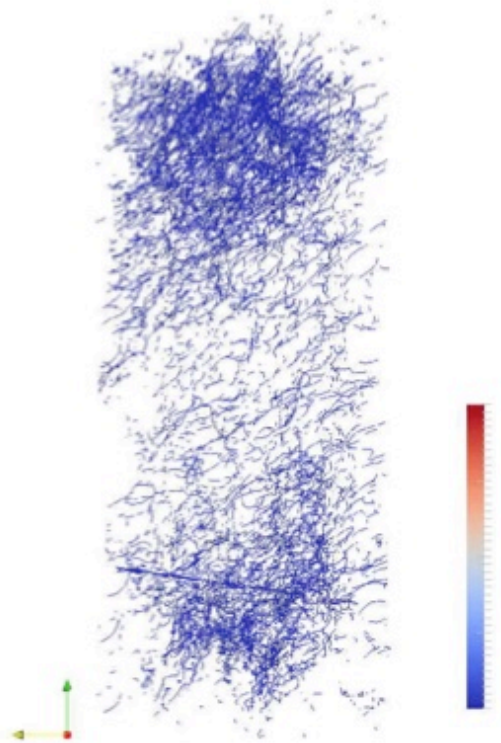
<001> Ni parameters; 20 x 20 x 50 μm simulation cell;
surface, intersection and 'bulk' cross slip included



Initial condition
ρ_o = ~2 x $10^{11}/m^2$



(-111)[101]
Slip system



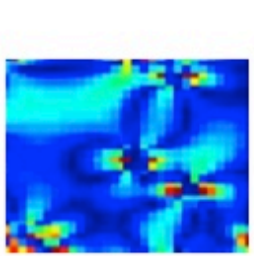
(1-11)[011]
Slip system

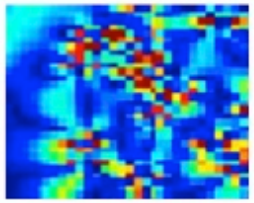
S.I. Rao, et al., (2015- present)
A. Hussein, et al. (2015- present)

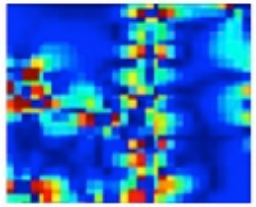
The physics is missing for handoffs to higher scales!

Hierarchies of Correlation Length Approximations*

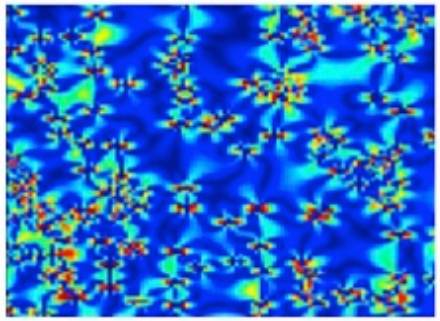
$$R_{xx}(l_1,l_2) = \int\int x_1 x_2 f_{x(l_1)x(l_2)}(x_1,x_2)dx_1 dx_2$$

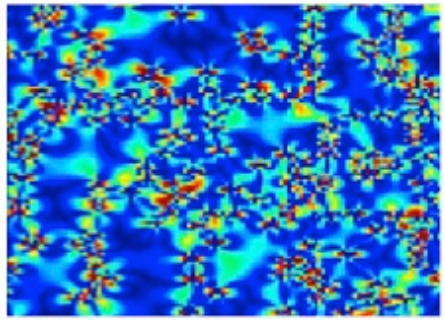




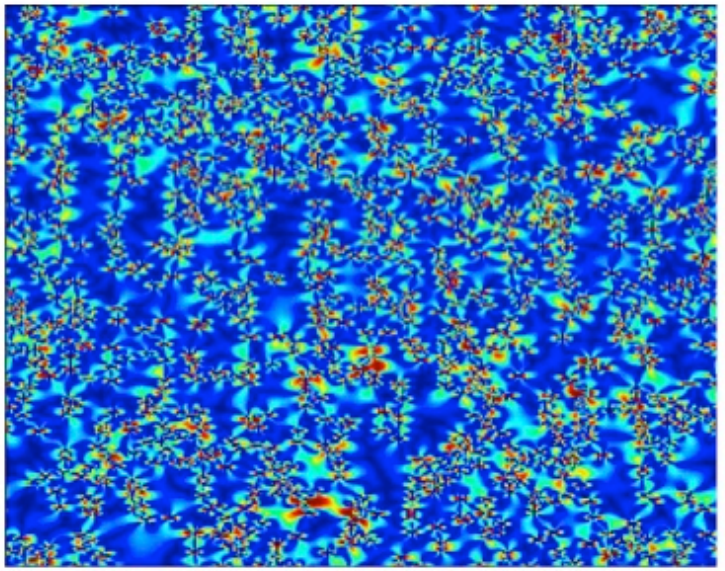


a_3

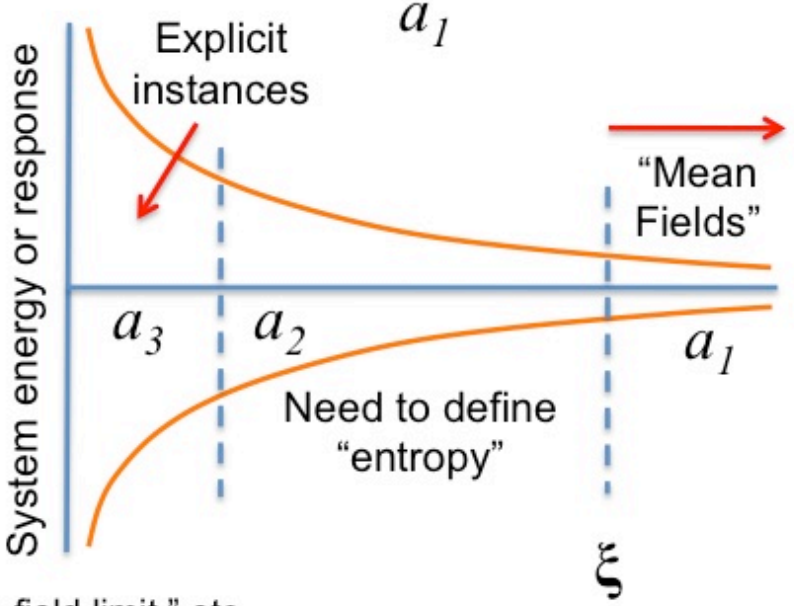




a_2



a_1



Adapted from:
I. Simonovski, M Kovac & L. Cizelj, MSEA 381 (2004)
V. Bedichevski & DM Dimiduk, Scripta Mater. 52 (2005)
V. Bedichevsky, Scripta Mater. (2006)
M-C. Miguel, et al, Eur Phys Jol B, 64 (2008)

*also called, "de-correlation length," "coherence length," "mean-field limit," etc.

Correlated Microstructure Effects

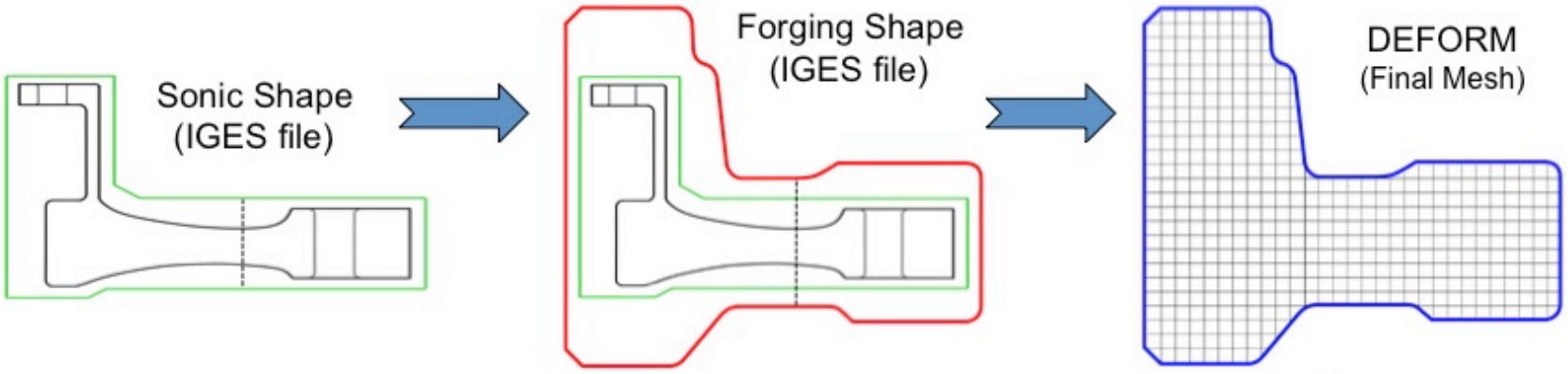
- Atom-atom, dislocation-dislocation, particle-particle, fiber-fiber, grain-grain, ply-ply, etc. *Local interactions control the stresses that matter*, not the far-field stresses

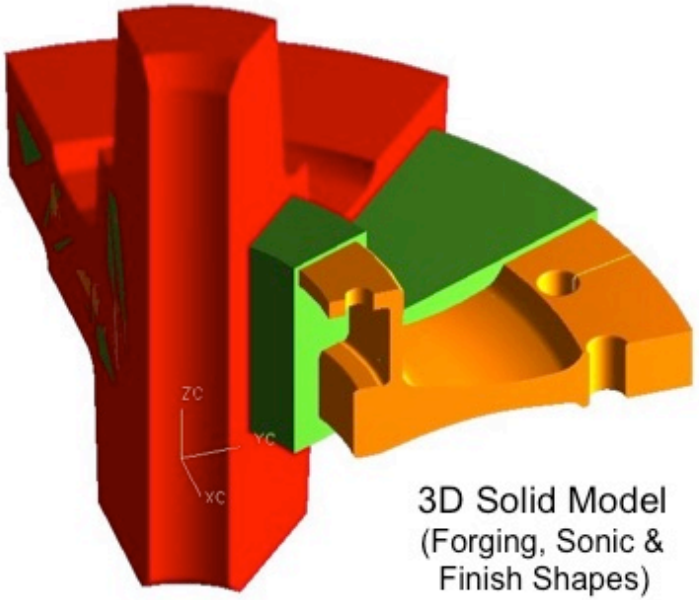
- More precisely, the multi-axial, far-field mechanical state is always mapped into *a spectrum of local kinematics states via the non-linear, hierarchical prism of "microstructure"…*

- Hypothesis of *"scale separation"* is the only reason we can simulate and predict the little that we can, but *how do we objectively separate scales?*...

- Therefore, it is essential to *objectively define probabilities of* mean-fields or *continuum fields at each scale*, in space and time… *via quantitative correlation lengths*…

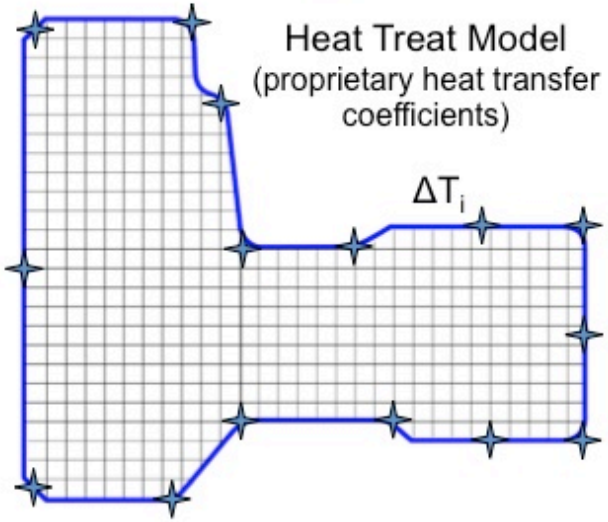
Forging Supplier: Forging Design & Modeling





3D Solid Model
(Forging, Sonic & Finish Shapes)

Return IGES File of Results to OEM for Approval



What do we place at each node to compute properties in this workflow?

Analytical Models for Al vs TiAl Alloy ICME

Temperature, Time & Composition-Dependent Yield Strength Model for Al-Alloy ICME

S. Weakley et al., *Met. and Matls. Trans. A*, 35A (2004), p. 2407

$$\sigma_Y(T,t,c) = \sigma_{ppt}(T,t,c) + \sigma_{GP/ss}(T,t,c) + \sigma_i$$

$$\sigma_{ppt}(T,t,c) = M(0.13\left\{\frac{Gb}{\sqrt{dw}}\right\}\left\{\sqrt{f} + 0.75\sqrt{\frac{d}{w}}f + 0.14\frac{d}{w}f^{3/2}\right\}\left\{\ln\frac{0.87\sqrt{dw}}{r_o}\right\})$$

$$\sigma_{GP/ss}(T,t,c) = A\left(c_o - \frac{f}{3}\right)^{2/3}$$

$$\sigma_i = 70MPa$$

For Virtual Aluminum Casting

Grain & Lamellae Size Dependent Yield Strength Model for Fully Lamellar TiAl Alloys

D.M. Dimiduk, et al., *Met. and Matls. Trans. A*, 29A (1998), p. 45

$$\sigma_Y = \sigma_{reference} + \sigma_{lamellae} + \sigma_{grains}$$

$$\sigma_Y = M_s\left\{\tau_o + \left[4\tau_2 * \mu b/\alpha\pi\lambda(D)\right]^{1/2} + \left[(2-\nu)\pi\tau_3 * \mu b/2(1-\nu)D\right]^{1/2}\right\}$$

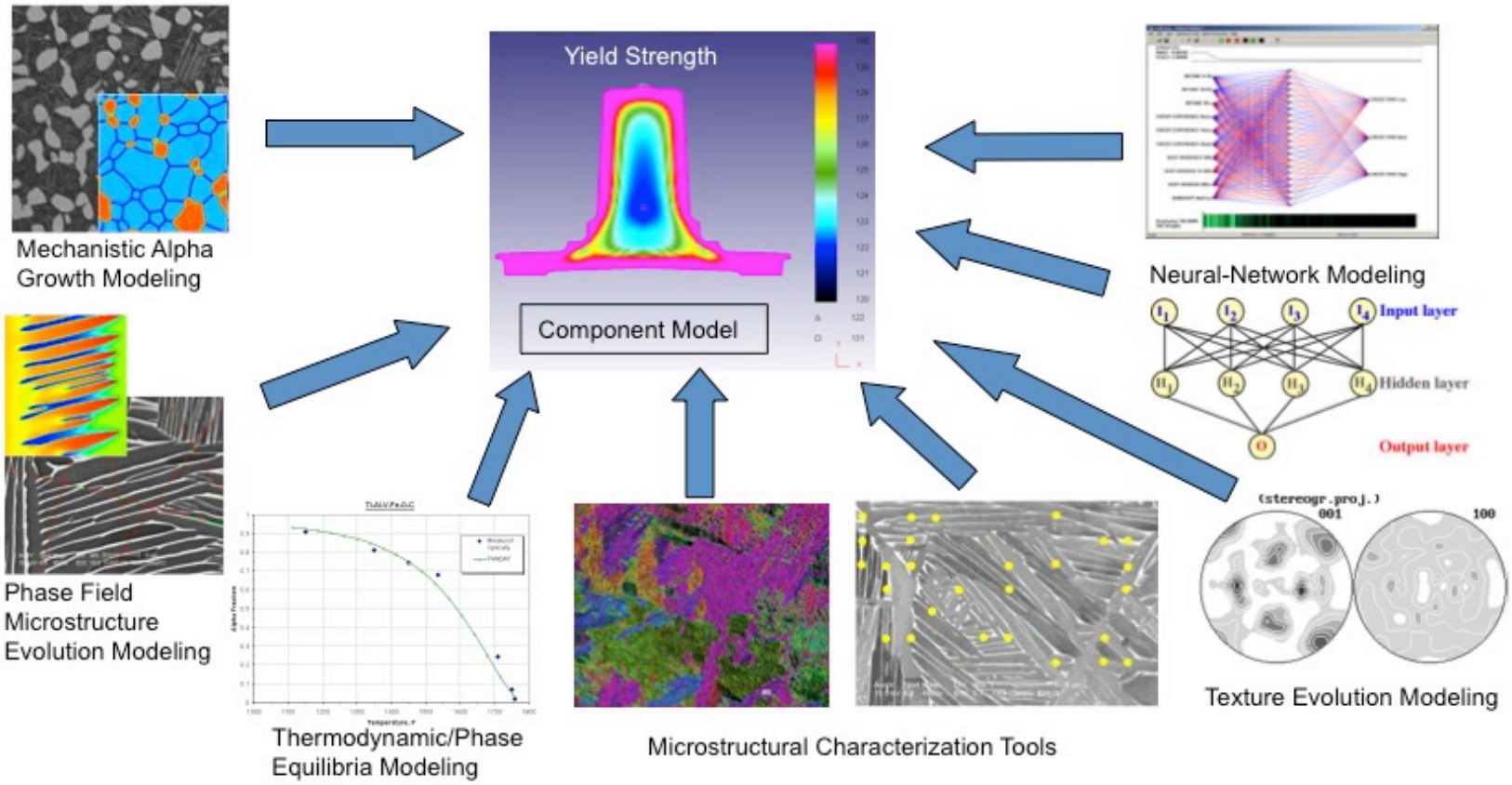
$$\sigma_Y = A + B/D^{1/4} + C/D^{1/2}$$

where A = 175 MPa, B = 70 MPa-m$^{-1/4}$, and C = 1 MPa-m$^{-1/2}$

Only microstructure variables, no temperature, time or composition

Analytical models offer significant compute-time advantages for process optimization

Titanium Alloy Modeling Framework
(Analogous Frameworks for Al, Ni,… Alloys)

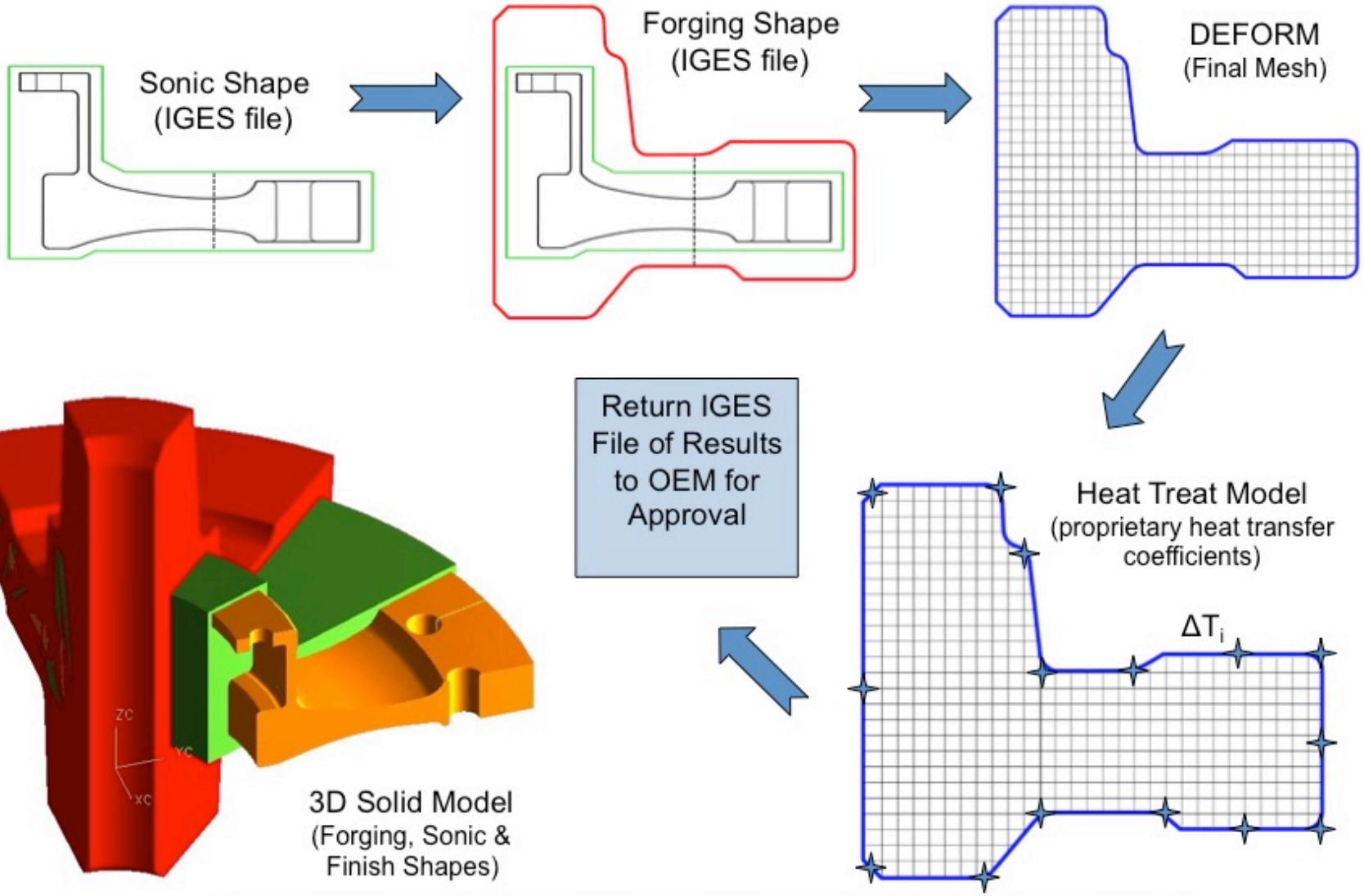


Microstructure and Mechanical Property Tools are being Developed and Utilized in Combination to Predict Structures/Properties in Components

Furrer, et al., (2005 – present)

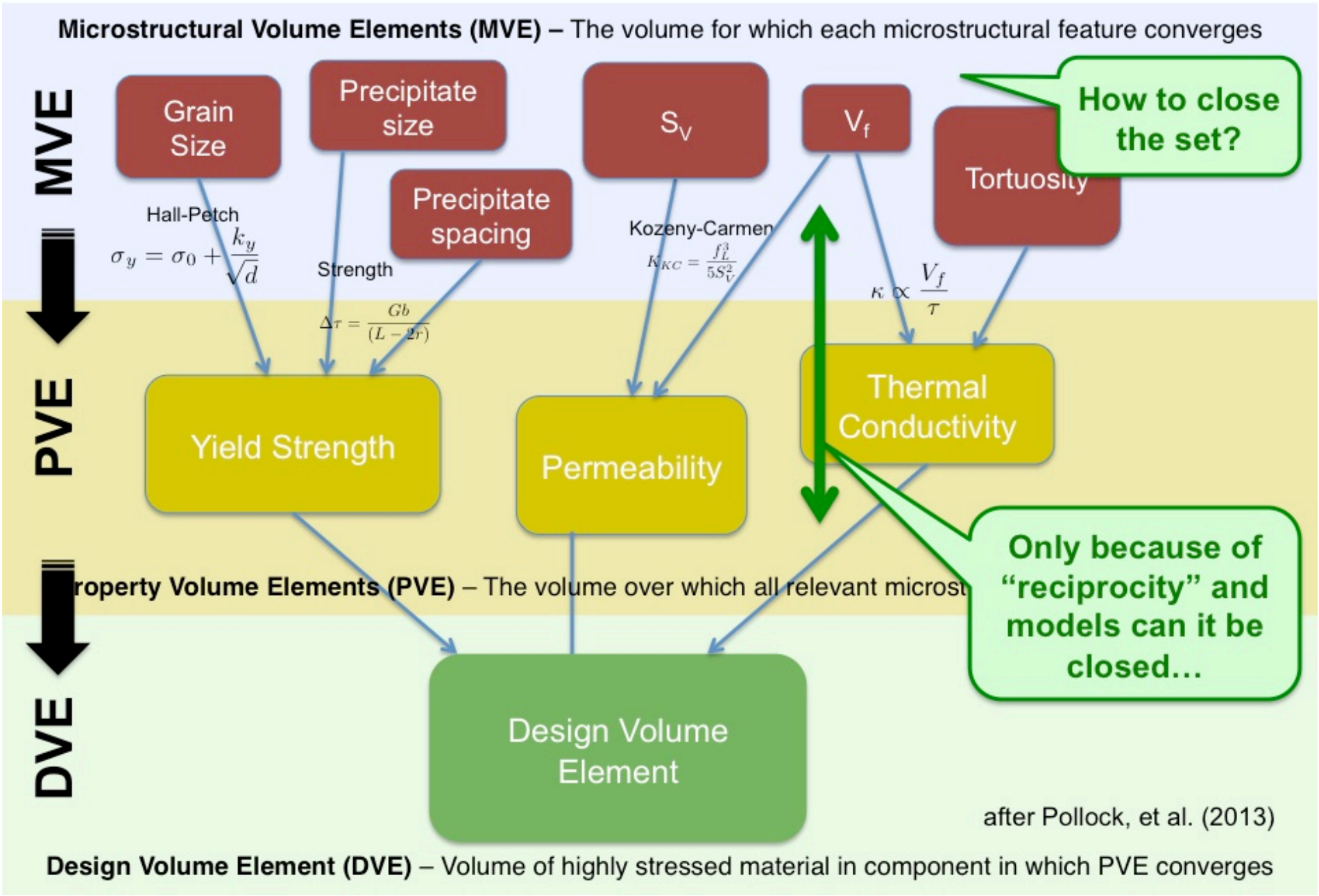
See also M.G. Glavicic and V. Venkatesh, *JOM* (2014); D. Wang, R. Shi, Y. Zheng, R. Banerjee, H. Fraser and Y. Wang, *JOM* (2014)

Forging Supplier: Forging Design & Modeling

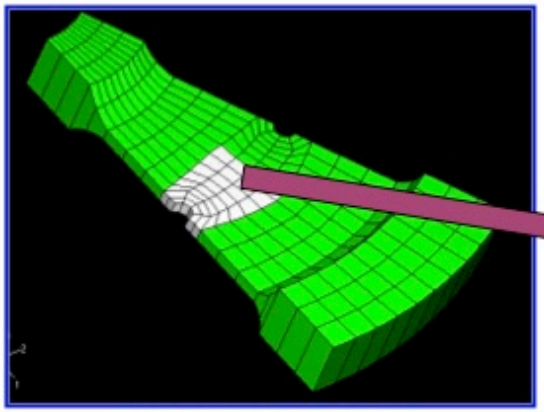


We want an RVE or SERVE at each point, for cause!

A Perspective on Representative Volumes



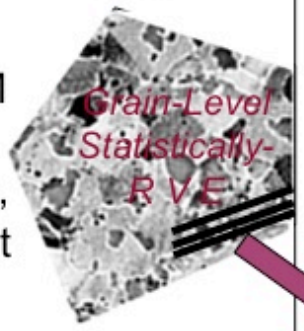
The "Plasticity Engine" for Properties



Design Concept

Define Features

Multiaxial FEM Analysis Of Polycrystalline, Polyconstituent Material

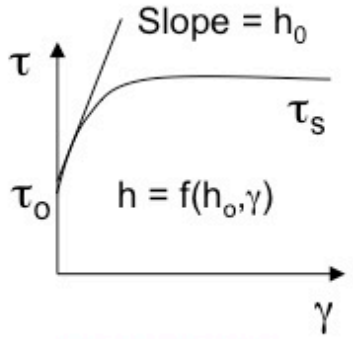


Plastic Heterogeneity & Strain Localization

Focus on Work-Hardening Parameterization *With μ/s Effects*

$$\dot{\tau} = \left\{ h - \left(\frac{\tau - \tau_o}{\tau_s - \tau_o} \right) h \right\} \left(\dot{\gamma} / \dot{\gamma}_o \right)^m$$

Properties of Representative Volume Element



Conventional "J_2" Finite Element Model	$\{\tau_o, \tau_s, m, h\}$
Continuum Crystal Plasticity	$\{\tau_{o,i}, \tau_{s,i}, m, h_{ij}\}$
Constrained Crystal Plasticity	$\{\tau_{o,i}(k_{hp}), \tau_{s,i}, m, h_{ij}\}$
Strain-Gradient Crystal Plasticity	$\{\tau_{o,i}, \tau_{s,i}, m, h_{ij}\} + k_o$

must define $\tau(\rho)$, $\rho(\gamma)$ to find k_o

increasing granularity & compute complexity

Parthasarathy & Dimiduk, et. al. (2000 -)

von Mises or "J_2 Plasticity"
The Work Horse Methods for Structures Analysis

"Second invariant of the stress" defined as

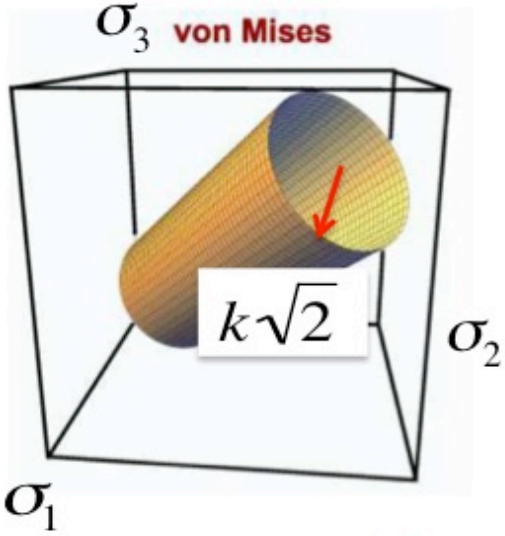
$$J_2 = \frac{1}{6}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]$$

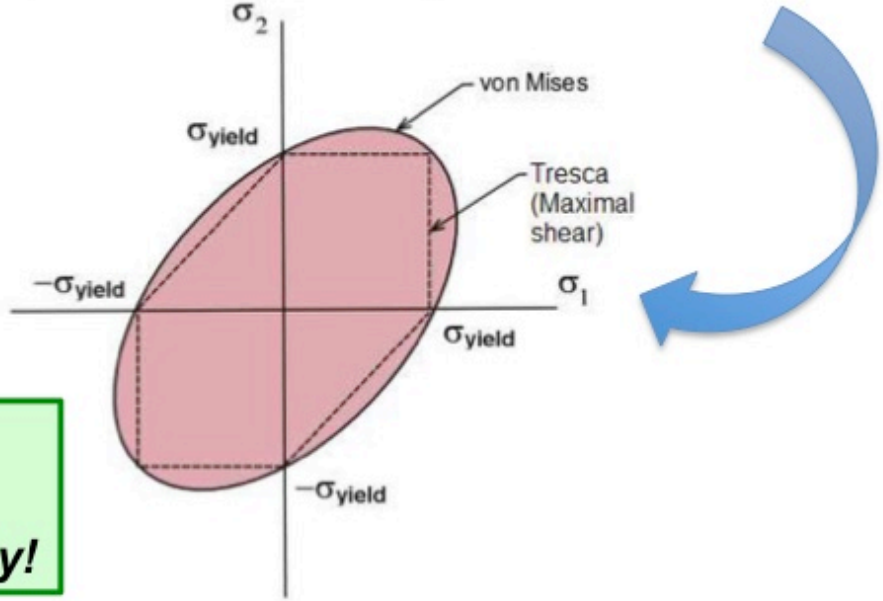
Plastic flow begins when J_2 is equal to some "yield function" k^2

$$\frac{1}{6}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right] = k^2$$

For Plane Stress, σ_3

$$\frac{1}{6}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2)^2 + (\sigma_1)^2\right] = k^2$$





How to obtain yield functions?
Must account for strain hardening
Yield function evolves heterogeneously!

Selected Finite Element Codes

Some Professional Codes for Structures Analysis:

- ANSYS
- ABAQUS
- MARC
- LS-DYNA (for dynamics)

All have “built-in” materials models and ability to link to measured “allowables”
Most have capability for “User Material Subroutines” (UMATs)
“non-Local” methods are not standardized, and mostly unavailable

Open Source Frameworks Emerging

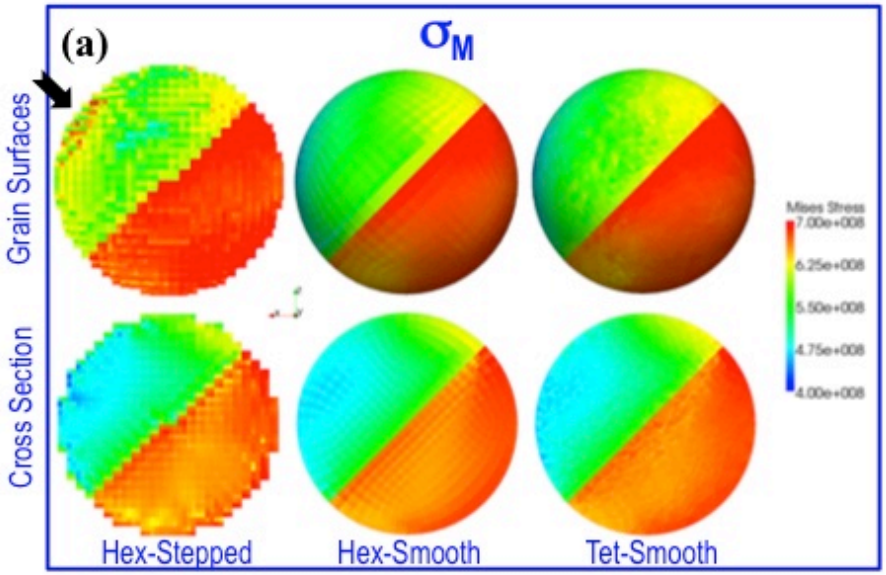
- Idaho National Laboratory: http://mooseframework.org/
- Sandia National Laboratory: https://software.sandia.gov/albany/
- Others

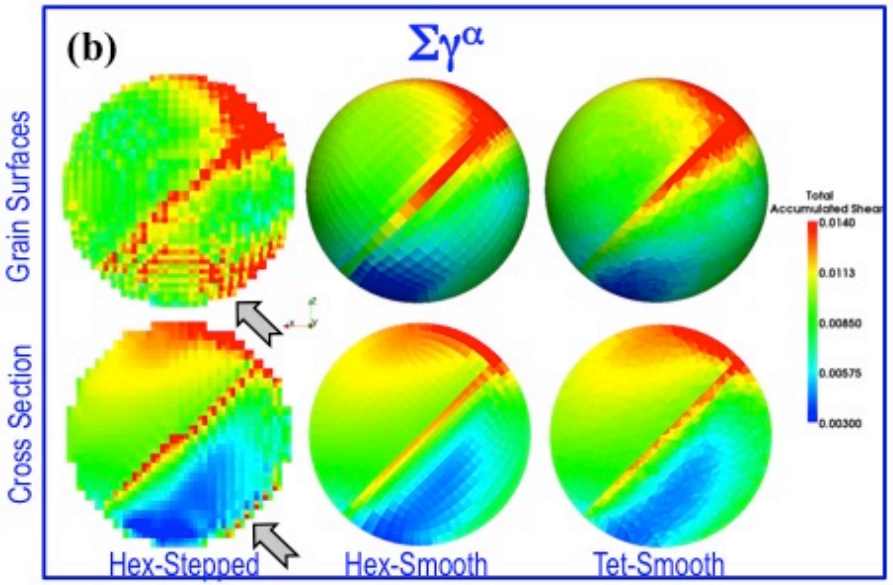
No codes are designed for the unique challenges of materials engineering!

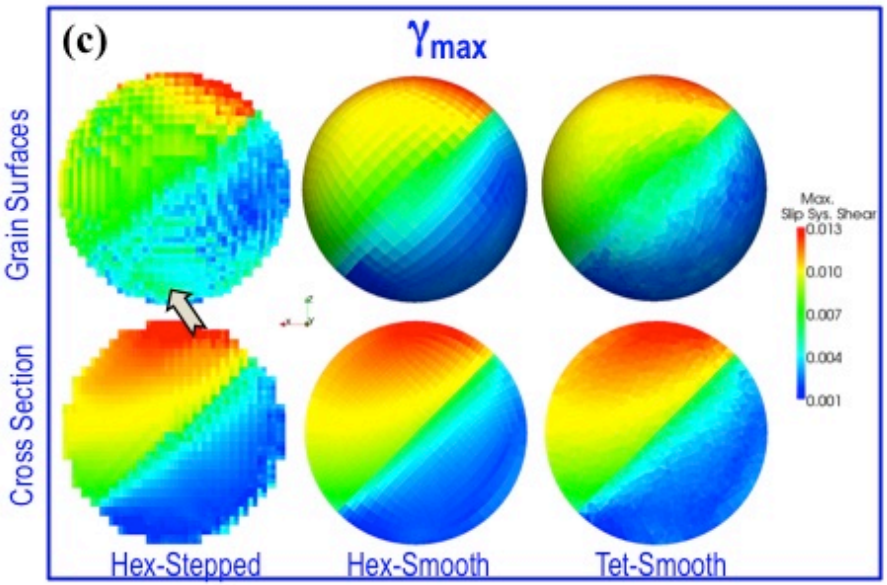
Historically, codes have terrible compute scaling (even worse licensing…)

All require materials models, most require meshes…

Numerical Limitations: Meshing Effects







Bicrystal spheres visualized by

(a) σ_M, von Mises effective stress

(b) $\Sigma\gamma^\alpha$, sum of shears on individual slip systems

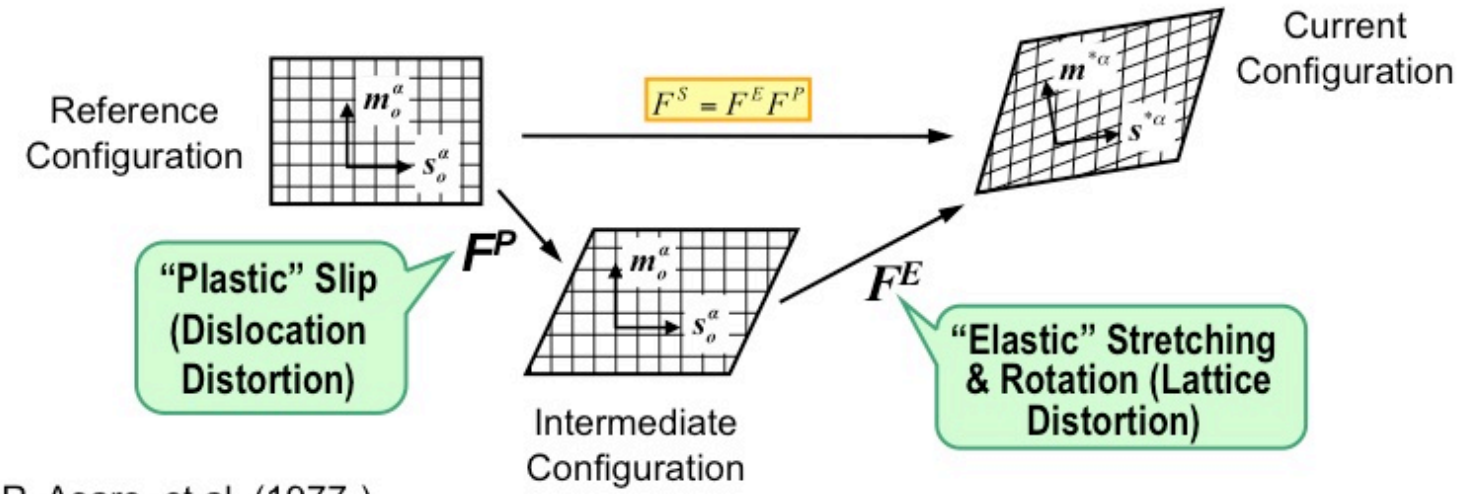
(c) $\gamma^\alpha{}_{max}$, maximum shear strain on any slip system

for the hex-meshed stepped, hex-meshed smooth and, tet-meshed smooth cases.

Choi, et al., MSEA, 553 (2012) p. 37

A "Local" Crystal Plasticity Model: Kinematics

A Familiar Diagram from Crystal Plasticity Mechanics



after R. Asaro, et al. (1977-)

Basic Equations Representing Material

$$\mathbf{L}^{\mathrm{P}} = \sum_{\alpha} \dot{\gamma}^{\alpha} \left(\mathbf{s}_o^{\alpha} \mathbf{m}_o^{\alpha} \right)$$

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_o \operatorname{sgn}(\tau^{\alpha}) \cdot \left| \frac{\tau^{\alpha}}{\hat{g}^{\alpha}} \right|^{1/m}$$

$$\hat{g}^{\alpha} \propto \hat{g}_o + \eta \mu b \sqrt{\rho}$$

Plastic flow is sum of *homogenized* slip rates

Slip rates follow *power law* of effective stress

Slip resistance given by *forest law*

Crystal Plasticity Finite Element Method

From dislocation motion to homogenized constitutive models

- Kocks, Argon, Ashby, *Prog. Mater. Sci.*, 19 (1975) p. 1
- Teodosiu, et al., (circa mid 1970's)
- Kocks & Mecking, *Prog. Mater. Sci.*, 48 (2003) 171

The CP-FEM method

- Asaro, R. J. and Rice, J. R., *J. Mech. Phys. Solids*, 25 (1977) p. 309
- Peirce, D., Asaro, R. J. and Needleman, A., *Acta metall.*, 31 (1983) p. 1951

Deeper background and current practitioners

- A. Needleman, *Acta Mater.*, 48 (2000) p. 105
- J. Harder, *Int. Jol. Plast.*, 15 (1999) p. 605
- P. Dawson, et al., R. Becker, et al. (1980's – present)
- G. Cailletaud et al., D. Parks, et al. (circa mid 1980's – late 1990's)
- D. McDowell, et al., S. Ghosh, et al. (mid 1990's – present)
- R. Lebensohn, et al. (mid 1990's – present)
- C. Hartley, *Phil. Mag.*, 83 (2003) p. 3783
- Y.-S. Choi & R. Brockman, Ch 6 in "Computational Methods for Microstructure-Property Relationships," S. Ghosh and D.M. Dimiduk, eds., Springer (2011)
- Many others

Simplest Crystal Plasticity Modeling

A Typical Flow-Rate Equation

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

Power Law Flow

Example Hardening Equations

Hardening Tied to Storage & Recovery (Kocks-Mecking-Estrin)

$$\hat{g} - \hat{g}_o = \eta \mu b \sqrt{\rho}$$

$$\dot{\rho} = \sum_{\alpha=1}^{n} \left[k_1 \sqrt{\rho} - k_2(\dot{\varepsilon}, T)\rho \right] \left| \dot{\gamma}^{\alpha} \right|$$

$$\dot{\hat{g}} = \left[k_1 \frac{\eta \mu b}{2} - k_2 \frac{(\hat{g} - \hat{g}_o)}{2} \right] \cdot \sum_{\alpha} \left| \dot{\gamma}^{\alpha} \right|$$

Isotropic Hardening Approximation

$$\dot{\hat{g}} = \theta_{II} \left(\frac{\hat{g}_s - \hat{g}}{\hat{g}_s - \hat{g}_o} \right) \cdot \sum_{\alpha} \left| \dot{\gamma}^{\alpha} \right|$$

For Anisotropic Hardening

$$\dot{\hat{g}} = \sum_{\beta=1}^{n} h_{\alpha\beta} \left| \dot{\gamma}^{\beta} \right| \quad \text{where} \quad \begin{matrix} h_{\alpha\alpha} = F(\gamma^{\alpha}) A(\gamma^{\beta}) \\ h_{\beta\alpha} = q h_{\alpha\alpha} \end{matrix}$$

self hardening *interactions*

FFT Numerical Method
Its Scalable and "Open Source" Code(s) Exist

- R. Lebensohn, F. Roters, P. Eisenlohr, et al. code: http://damask.mpie.de/Home/WebHome
- Expands deformation into a mean-field and a fluctuating spectral field solved in Fourier space
- The usual shortcomings of constitutive laws, both local and non-local —generally, constitutive laws are missing physics!
- Elasto-Viscoplastic, finite strain formulation (read metal working)
  - Excellent for large strains; deformation trending toward homogeneity
- Questionable accuracy for problems containing singularities…
  - Cracks, damage evolution, perhaps selected grain boundaries, etc.
- So far, no FEM code matches FFT method for speed, scaling or ability to examine microstructure statistics

Acharya-Beaudoin: "Non-Local" Length-Scale

- Evolution of $\rho_{\wedge}$ (*modified from the model of Kocks, Mecking and Estrin*)

$$\dot{\rho} = \sum_{\alpha} \left[k_o \left(\frac{\lambda^{\alpha}}{b} \right) + k_1 \sqrt{\rho} - k_2(\dot{\varepsilon}, T)\rho \right] \left| \dot{\gamma}^{\alpha} \right|$$

$\frac{1}{L'}$ L': Mean free path

$k_o(\lambda^{\alpha}/b) \Rightarrow$ Contribution of lattice incompatibility. → Mean free path $\propto \frac{1}{\lambda^{\alpha}}$

$k_1\sqrt{\rho} \Rightarrow$ Increment of ρ due to statistical $\perp$ forests. → Obstacle spacing $\propto \frac{1}{\sqrt{\rho}}$

$k_2(\dot{\varepsilon}, T)\rho \Rightarrow$ Dynamic recovery of $\perp$.

- Empirical Relation (*by Bailey and Hirsch*)

$$\hat{g} - \hat{g}_o = \eta \mu b \sqrt{\rho}$$

"extra" hardening from Curl L^p of gradient field couples to boundary conditions

- Description of Hardening

$$\dot{\hat{g}} = \frac{\eta^2 \mu^2 b}{2(\hat{g} - \hat{g}_o)} k_o \sum_{\alpha} \lambda^{\alpha} \left| \dot{\gamma}^{\alpha} \right| + \theta \sum_{\alpha} \left| \dot{\gamma}^{\alpha} \right|$$

$$\theta = \theta_o \left(\frac{\hat{g}_s - \hat{g}}{\hat{g}_s - \hat{g}_o} \right)$$

A Acharya & A Beaudoin, JMPS, 48 (2000) p. 2213; A Beaudoin, A Acharya, et al, Acta Mater. 48 (2000) p. 3409

Ma, Roters et al.: Signed Dislocation Density Model

Widely Used Non-local Model for SSD and GND Densities

$$\rho_f^\alpha = \sum_{\beta=1}^{N} \chi^{\alpha\beta} \rho_{SSD}^\beta \left|\cos\left(\mathbf{n}^\alpha, \mathbf{t}^\beta\right)\right| + \rho_{GNDs}^\beta \left|\cos\left(\mathbf{n}^\alpha, \mathbf{d}^\beta\right)\right| + \rho_{GNDet}^\beta \left|\cos\left(\mathbf{n}^\alpha, \mathbf{t}^\beta\right)\right| + \rho_{GNDen}^\beta \left|\cos\left(\mathbf{n}^\alpha, \mathbf{n}^\beta\right)\right|$$

$$\rho_p^\alpha = \sum_{\beta=1}^{N} \chi^{\alpha\beta} \rho_{SSD}^\beta \left|\sin\left(\mathbf{n}^\alpha, \mathbf{t}^\beta\right)\right| + \rho_{GNDs}^\beta \left|\sin\left(\mathbf{n}^\alpha, \mathbf{d}^\beta\right)\right| + \rho_{GNDet}^\beta \left|\sin\left(\mathbf{n}^\alpha, \mathbf{t}^\beta\right)\right| + \rho_{GNDen}^\beta \left|\sin\left(\mathbf{n}^\alpha, \mathbf{n}^\beta\right)\right|$$

From these and previous equations:

7 or 8 fitting constants; $c_1 - c_8$ (Keshavarz & Ghosh use 7)

slip activation energy, diffusion energy; ΔH_{slip} & ΔH_{bulk} (perhaps also D_{bulk} & $\dot{\gamma}_{ref}$)

6 a teraction strength coefficients; (treat as isotropic?)

dip n distance; d_{dipole} (expand as dipole model stress)

…c ysics, certainly in superalloy gamma channels

Is this really "physics-based?"

For superalloys, this model leads to *12-17 "adjustable" parameters*, 1 - 3 matrix elastic constants, plus initial conditions (not discussed?), *for matrix-phase slip*…before particle cutting, looping or, shape, spacing and volume fraction effects of precipitates are considered… *what is the simulation sensitivity to these detailed terms?*

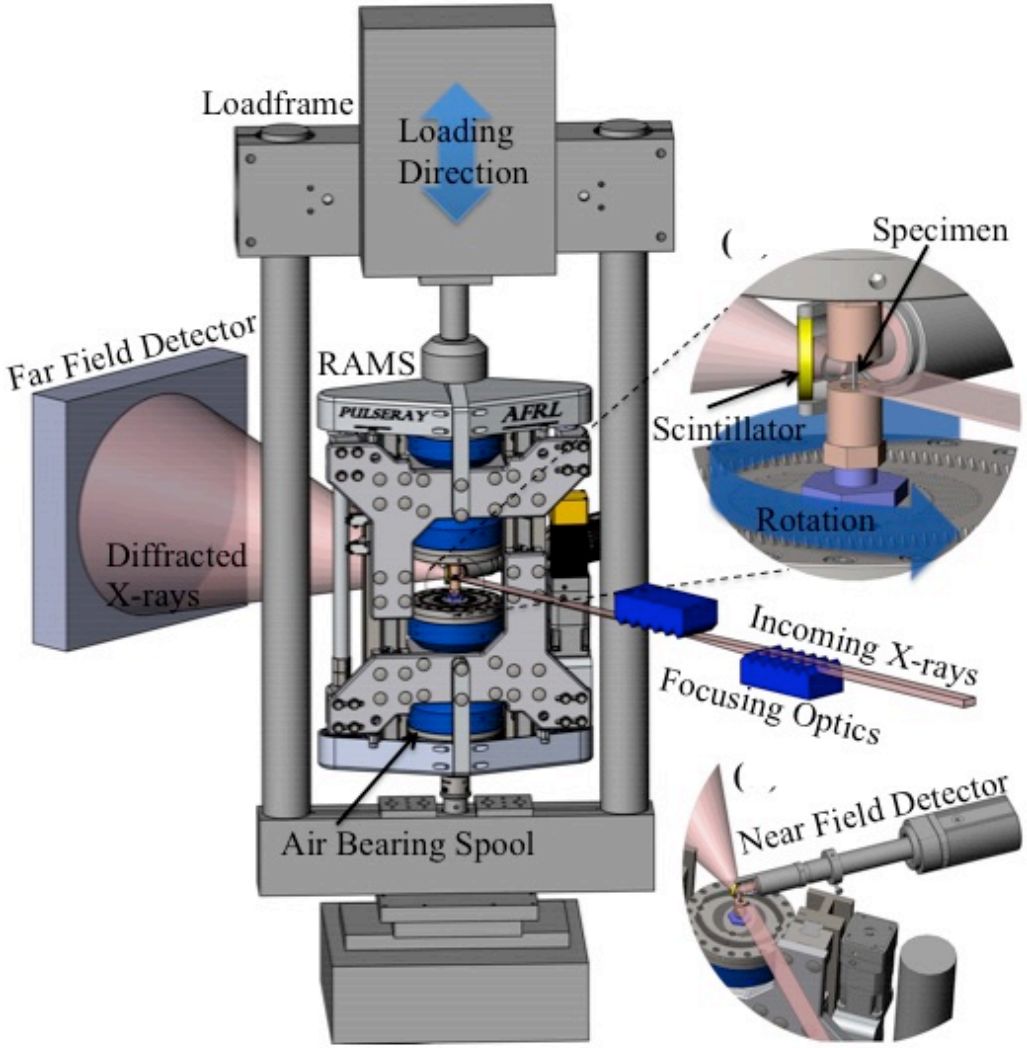
A. Ma and F. Roters, *Acta Mater.* (2004) p. 3603; A. Ma and F. Roters, D. Raabe, *Acta Mater.* (2006) p. 2169.

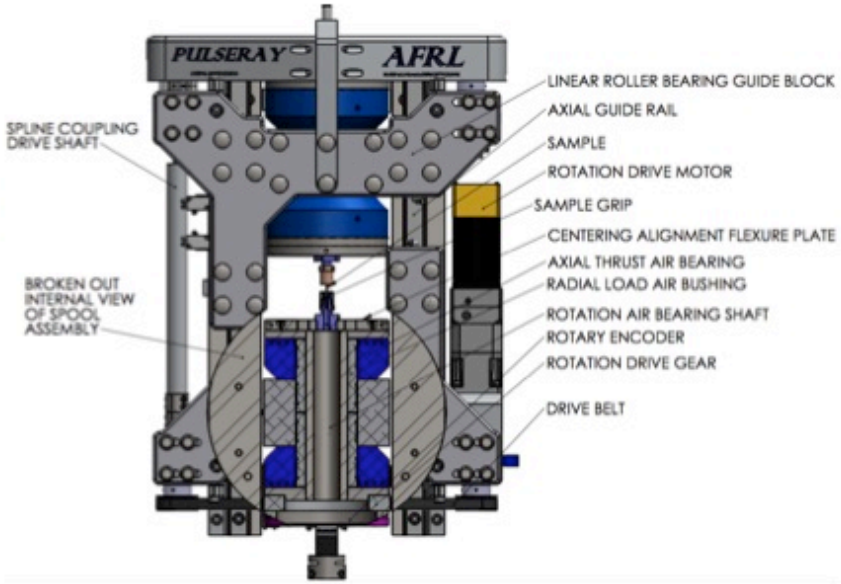
Other Non-Local, Emerging; Not Widely Available

- T. Arsenlis, et al. 1st signed dislocation densities model
- Acharya's (et al.) Field Dislocation Mechanics (FDM)
  - A. Beaudoin has generally functioning polycrystalline code
- El-Ezab's statistical mechanics method
  - Not published, only Anter knows…
- T. Hochrainer, M. Zaiser, et al., Continuum Dislocation Mechanics or "lift vector" method —a "4d" method is difficult, but course-grains both GND and SSD; theory not closed for density evolution
- I. Groma, et al., correlation function expansions…
  - Only 2d (1d)

- 3D dislocation ensemble physics still missing…
- Some are essentially computationally intractable
- Some retain the gradient length scale problem

Getting Closer to "Truth"…
High-Energy Diffraction Microscopy (HEDM)





J. Schuren, P. Shade et al., Current Opinion Solid State and Materials Science (2015)

Load Re-distribution Among Grains

Ti-7Al, Room Temperature Creep Stress

Von Mises Stress

$$\sigma_{eff} = \sqrt{\frac{1}{2}\begin{bmatrix}(\sigma_{xx}-\sigma_{yy})^2 + \\ (\sigma_{yy}-\sigma_{zz})^2 + \\ (\sigma_{zz}-\sigma_{xx})^2 + \\ 6(\sigma_{xy}^2+\sigma_{yz}^2+\sigma_{zx}^2)\end{bmatrix}}$$

Hydrostatic Stress

$$\sigma_H = (\sigma_{xx}+\sigma_{yy}+\sigma_{zz})/3$$

Applied Stress State

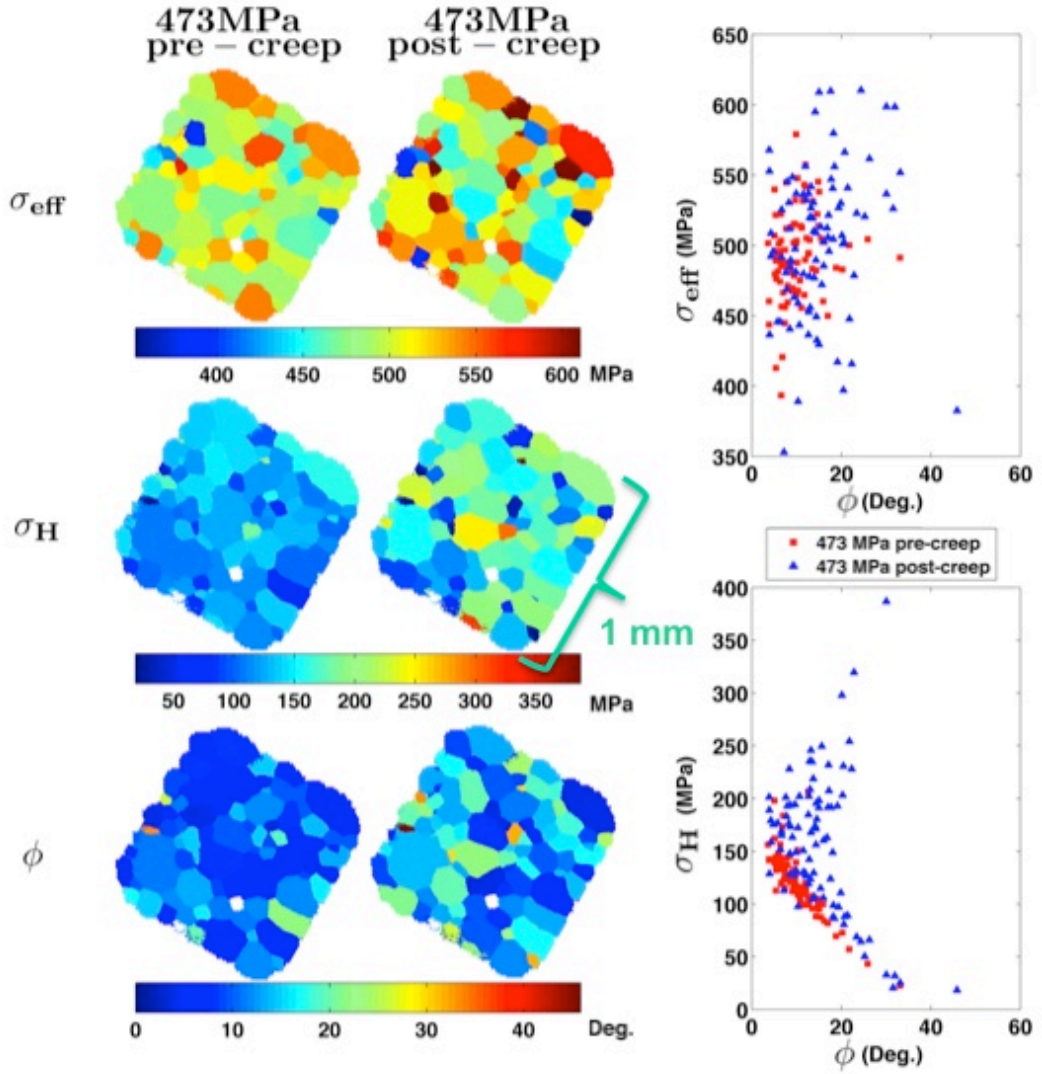
$$\bar{\sigma}_{axial} = [0,\sigma_{yy},0,0,0,0]$$

Grain Level Stress State

$$\bar{\sigma} = [\sigma_{xx},\sigma_{yy},\sigma_{zz},\sigma_{xy},\sigma_{xz},\sigma_{yz}]$$

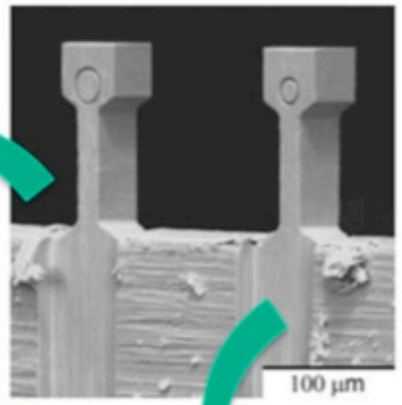
Co-axiality

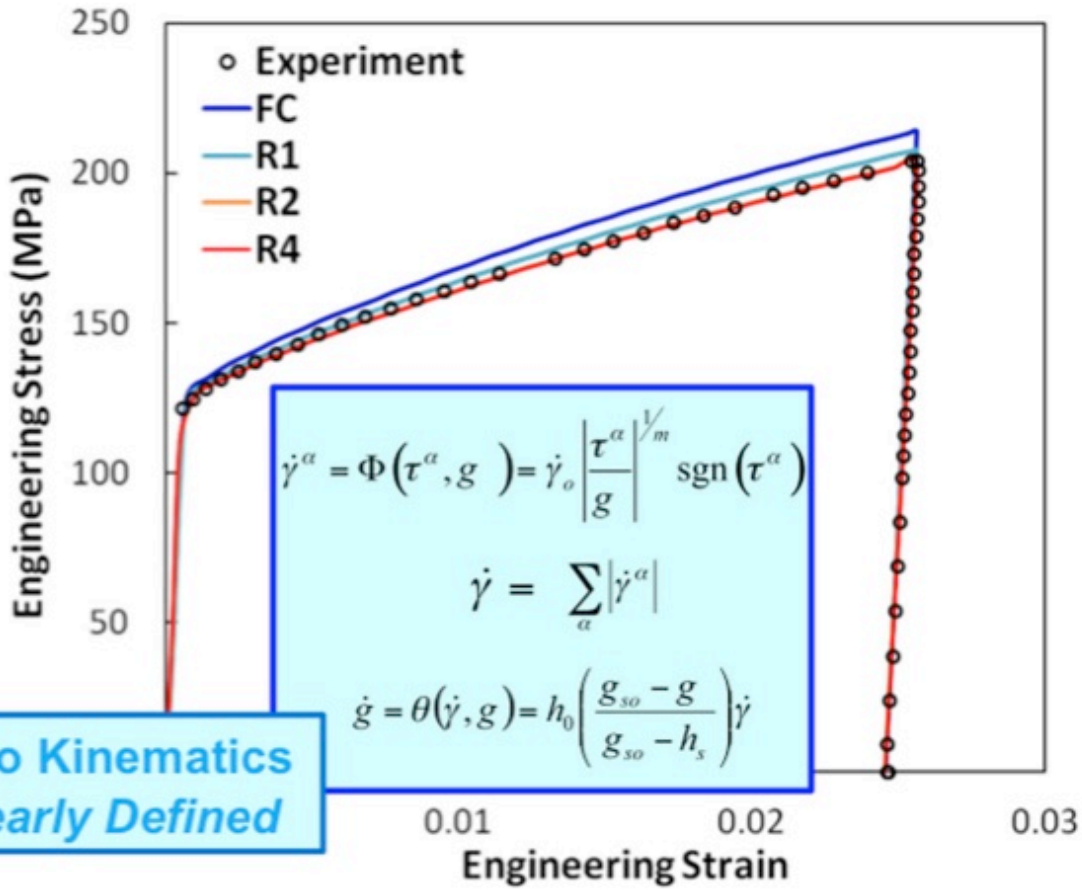
$$\phi = a\cos\left(\frac{\bar{\sigma}_{axial}\cdot\bar{\sigma}}{|\bar{\sigma}_{axial}||\bar{\sigma}|}\right)$$



J. Schuren, P. Shade et al., Current Opinion Solid State and Materials Science (2015)

Micro-Tension, Some Lessons Learned…





$$\dot{\gamma}^{\alpha} = \Phi\left(\tau^{\alpha}, g\right) = \dot{\gamma}_{o}\left|\frac{\tau^{\alpha}}{g}\right|^{1/m}\operatorname{sgn}\left(\tau^{\alpha}\right)$$

$$\dot{\gamma} = \sum_{\alpha}\left|\dot{\gamma}^{\alpha}\right|$$

$$\dot{g} = \theta\left(\dot{\gamma}, g\right) = h_{0}\left(\frac{g_{so} - g}{g_{so} - h_{s}}\right)\dot{\gamma}$$

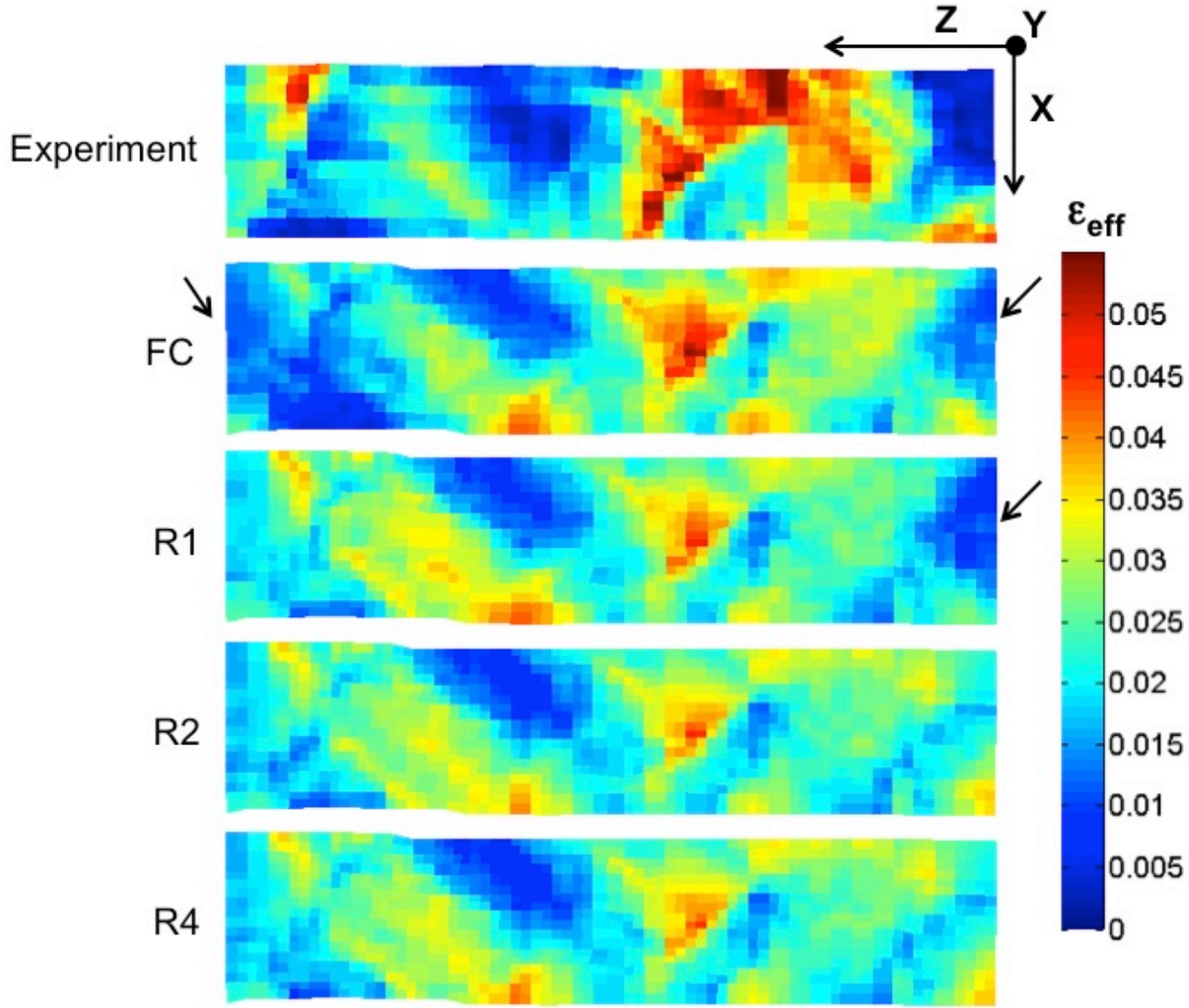
Limits to Kinematics
Not Clearly Defined

h_o	g_{so}	h_s	$g^{\alpha}_{initial}$	$\dot{\gamma}_0$	m
(MPa)	(MPa)	(MPa)	(MPa)	(s^{-1})	-
500	103	43	43	$1e^{-5}$	0.06

+/- Δ_{value} for each parameter value

Choi, Turner, Groeber, Schuren, Shade, et al. (2010 -); P. Shade, et.al., Intgr Mater. & Mfg. Innov., 2 (2013).

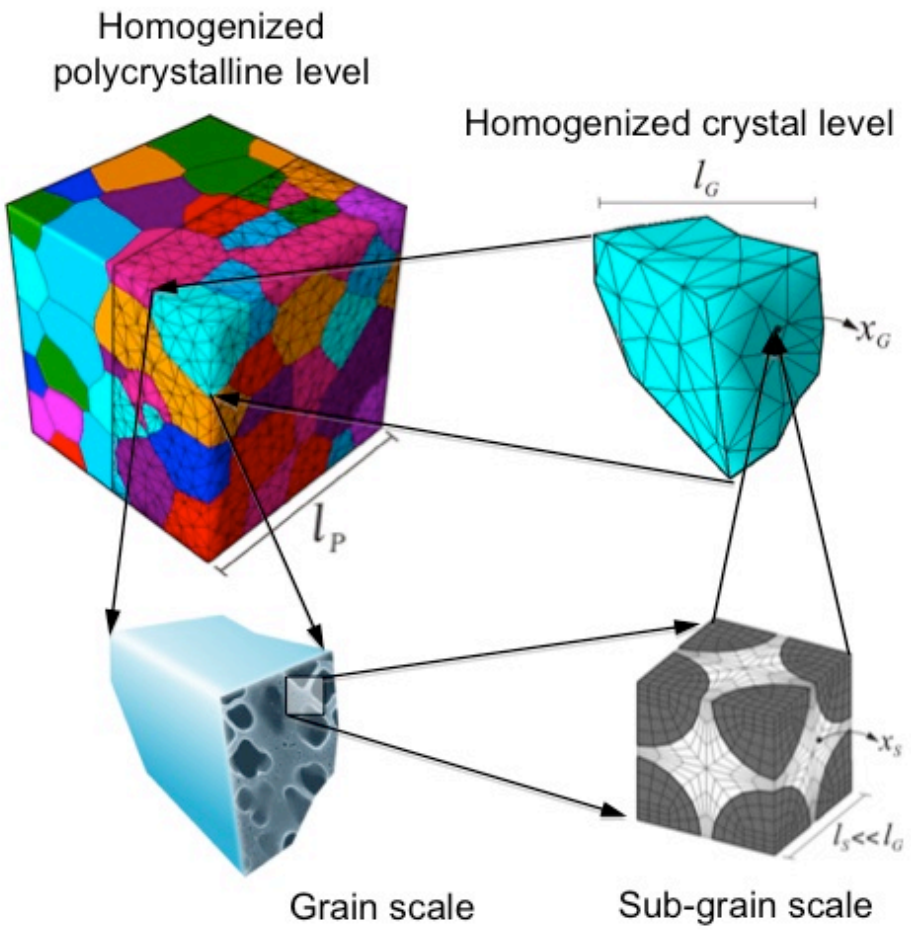
The von Mises Effective Strain after 2.5% Tension

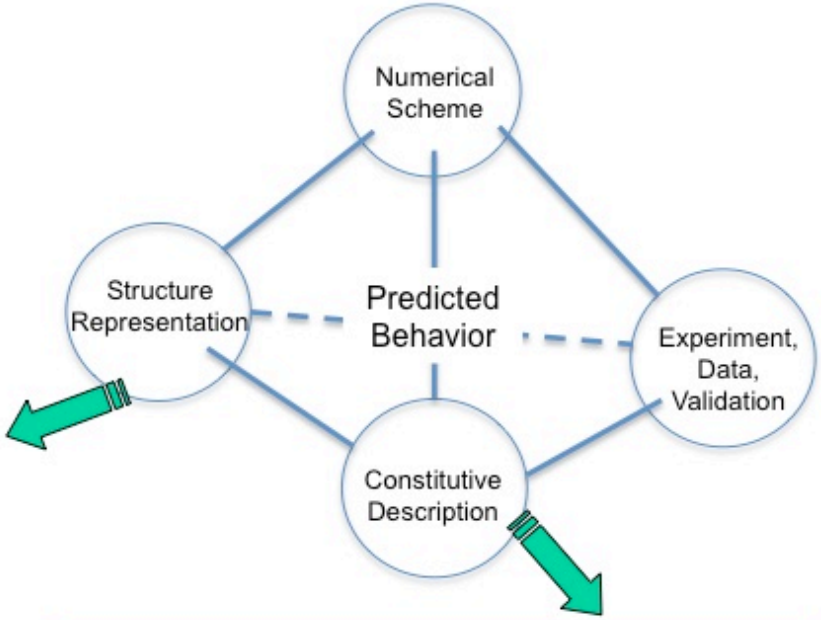


Experimental and simulated von Mises effective strains under different boundary conditions

Choi, Groeber, Shade, Turner, et al. (2010 -)

Then There is the Microstructure Problem…





$$\dot{\gamma}^{\alpha} = \dot{\gamma}_o \exp\left\{-\frac{\Delta H}{kT}\left(1-\left[\left[\frac{\left(\left|\tau^{\alpha}\right|-\tau_k^{\alpha}\right)}{\tau_o^{\alpha}}\right]^{p}\right]^{q}\right\}sgn(\tau^{\alpha})$$

$$\tau_o^{\alpha} = Gb\sqrt{\sum_{\beta=1}^{12} A_{\alpha\beta}\rho^{(\beta)}}$$

$$\dot{\rho}^{\alpha} = \frac{1}{bL^{\alpha}}\left|\dot{\gamma}^{\alpha}\right| - 2\frac{y_c}{b}\rho^{\alpha}\left|\dot{\gamma}^{\alpha}\right|$$

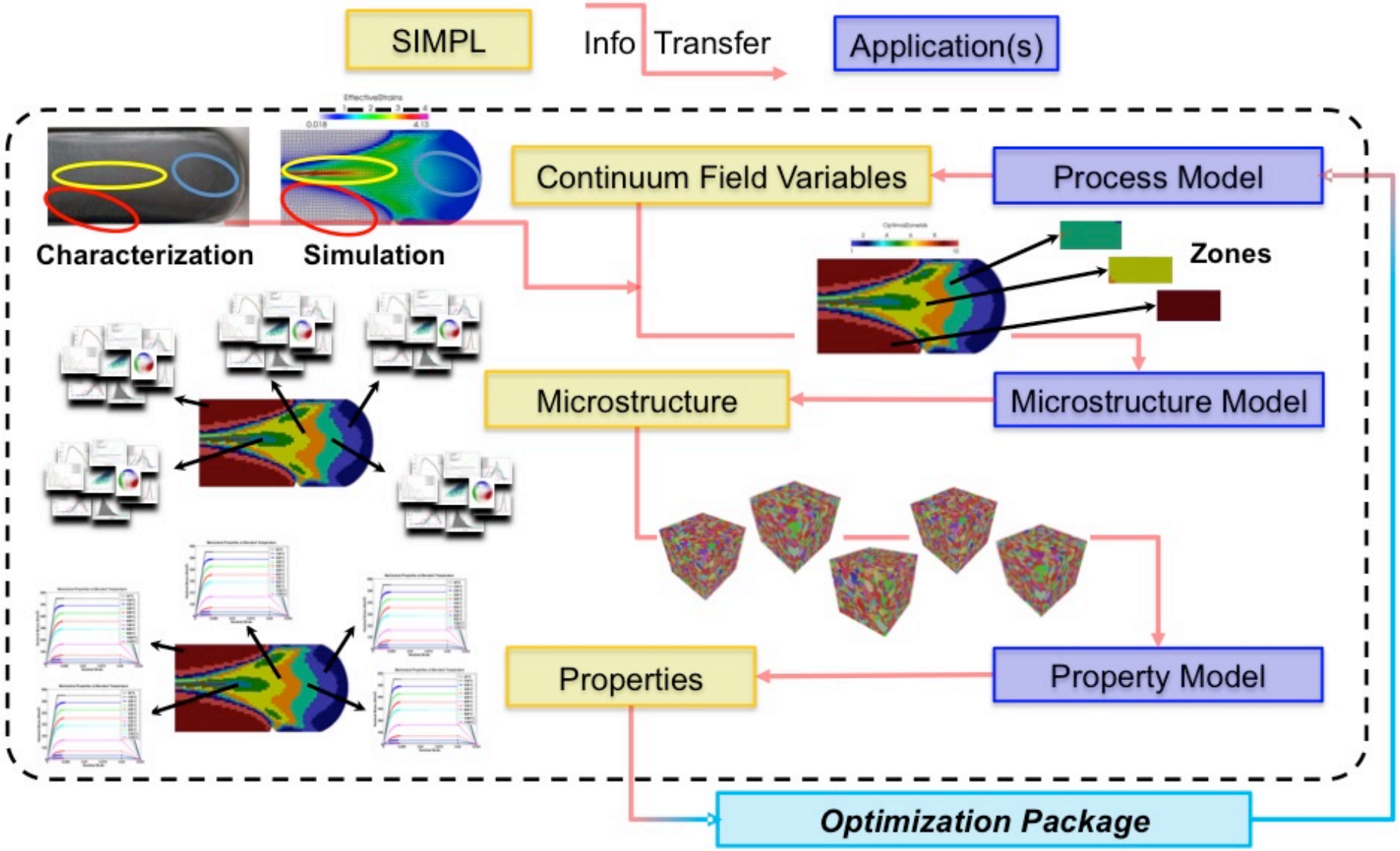
S. Ghosh and S. Keshavarz, (2013, 2014 -)

Consistency of constitutive models, microstructure hierarchy & discretization

Coarse-Graining RVE's: Back to Yield

- When all mesoscale models, simulations and understanding are in place, one still needs "fast-acting" frameworks for design and manufacturing optimization
- Usually precludes direct use of microstructure…
- Yield functions (with evolution) may work
  - Sophisticated analytical forms
  - examples
  - F. Barlat, Becker, et al., *J. Mech. Phys. Solids*, 45 (1997) pp. 1727-1763
  - F. Yoshida, H. Hamasaki, T. Uemori, *Int. Jol. Plast.*, 45 (2013) p. 113
- Digitally computed "look-up tables"
  - See S. Ghosh, et al.

Enabling Links to Engineering Design



DREAM.3D arbitrates model interactions & modularizes process

Integrated Design-Manufacturing-Materials