Multi-scale Modeling with MPM

Nuclear Fuel Pin Swelling During a Transient Event

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Outline

- **Problem Definition**
- **Why MPM?**
- **Validation Calcs**
  - plasticity
  - texture evolution under plastic deformation
- **MPM issues**

- **Goal of Talk: present a non-traditional application area for MPM**

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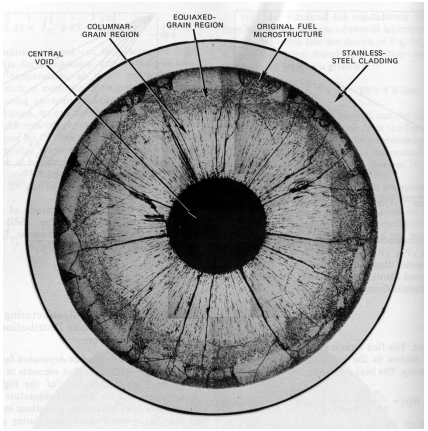
Goal & Strategy

- Develop a **validated and predictive** capability to simulate the mechanical response of a TRU fuel pin during a transient thermal event at the meso- to continuum scale.
  - **predict clad strain**

    initial focus: swelling due to fission gas inventory

    longer term: cracking (maybe??) (flow channels)



- **Strategy**
  - fission bubble transport dominated by vacancy distribution
    - atomic gas transport at interstitial sites: thermal diffusion --> $F_b = \left(\frac{2\pi R^3}{a_o^3} \right) \frac{Q^*}{T} \left(\frac{dT}{dx} \right)$
  - bubbles move up vacancy gradients
    - Evans, J.H., "Modelling of Fission Gas Bubble Migration to Grain Boundaries during Post-Irradiation Annealing of High Burn-up UO2", in Fission Gas Behaviour in Water Reactor Fuels, Nuclear Energy Agency, 2000.
  - extension to polycrystalline material with temperature and stress gradients
    - fuel pin

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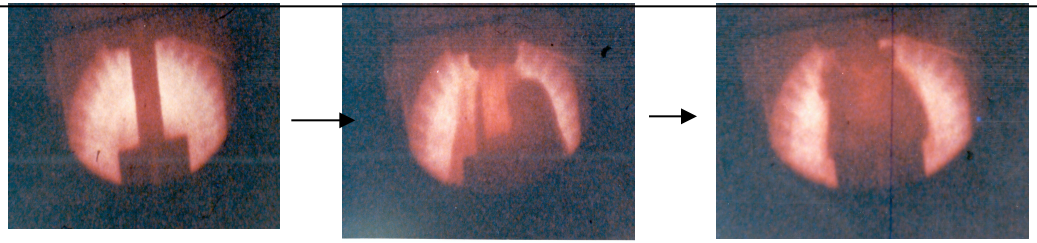
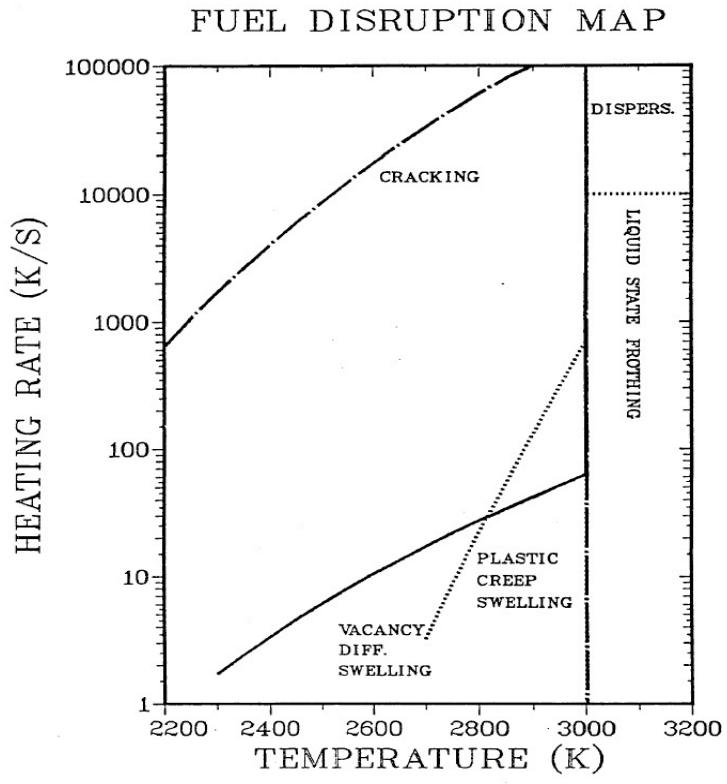
SNL – ACRR Reactor Experiments (MOX)
(1980's, Steve Wright, et. al.)



Pin heatup, clad melt and FP release, and fuel disruption sequence in LMFBR high burnup fuel pin (FD Program - PNC, UKAEA, KFK, NRC)



- Large difference between fresh and burned fuel transient response
- Why?
  - fission gas inventory
- Need for coupled in-pile & separate effects experiments and modeling/ simulation to understand.

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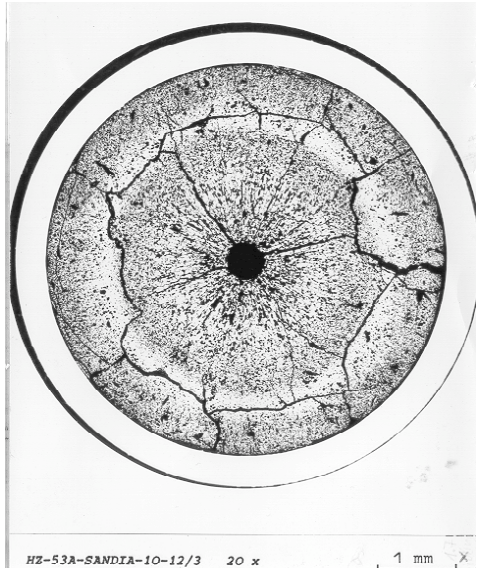
Fuel Pin Modeling Strategy: multiple length and time scales

Continuum Physics
- Lagrangian-MPM
  - -mechanical stress

MPALE

Mesoscale Physics
- Calibrated Monte-Carlo (CMC)
  - -texture evolution (Potts-Glauber)
  - -pore/bubble transport (Potts-Kawasaki)

Atomistic Physics
- Diffusion Theory
  - -energy (conduction)
  - -atomic structure
  - -atomic species
  - -gas clusters
  - -vacancies



why use MPM? Common data structures to facilitate information coupling:

MPM: particles and cells/grid

CMC: particle lattice

Diffusion: cells/grid

cracking???

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Coupling Challenges

- **MPM**
  - lagrangian MPM (small deformation….3-7% clad strains)
  - implicit mpp version (in progress)
  - discussion topics:
    - MPM vs single point FEM grids
      - multi-material interface issues
    - automatic multi-grid (similar to Fehlberg R-K?)

- **Diffusion**
  - it's the physics!
    - diffusivity as a function of temperature and strain gradient
    - using DFT (Density Functional Theory)

$$F_b = \left(\frac{2\pi R^3}{a_o^3} \right) \frac{Q^*}{T} \left(\frac{dT}{dx} \right)$$

- **cMC**
  - temperature dependent material constants
    - grain boundary energies, etc at elevated temperatures
    - example: Poisson ratio for PuO_2 ~ 1/3 @room temp; ~1/2 @elevated temp!

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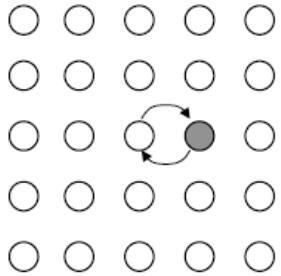
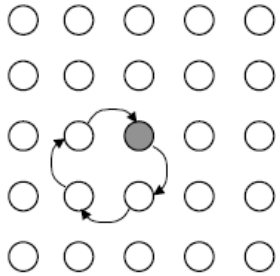
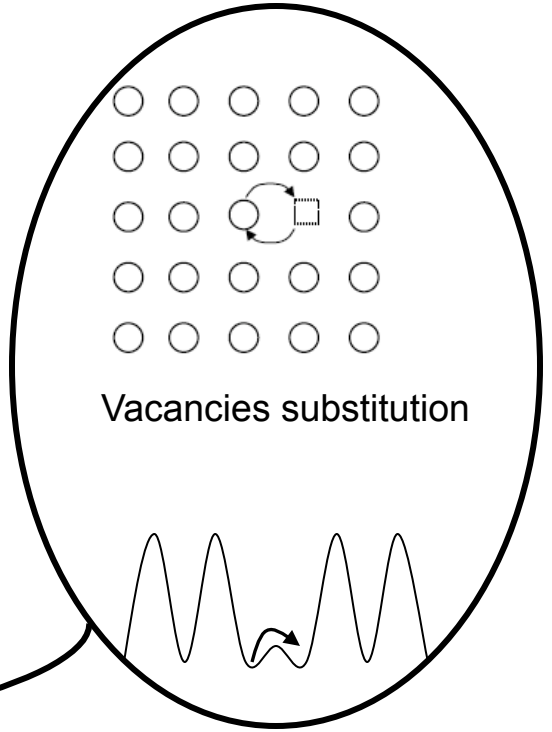
Atomic diffusion mechanism



Direct exchange



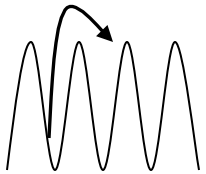
Ring mechanism
(all atoms rotate simultaneously)

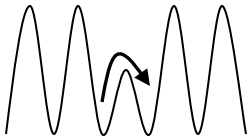


Vacancies substitution

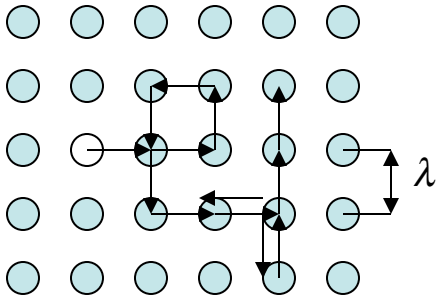
Probability to overcome energy barrier

$$p \propto \exp\left(\frac{Q}{RT}\right)$$





Random walk of vacancies through crystal lattice



Random walk sequence of a vacancy traveling in a lattice

Mean displacement after n steps
(Mean displacement null)

$$\langle \lambda_n \rangle = \frac{1}{k}\sum \lambda_k = 0$$

RMS
(Region where we can find walkers expands)

$$\sqrt{\langle \lambda_n^2 \rangle} = \sqrt{n}\lambda$$

Einstein equation: Diffusion is inherently related to atoms vibration around their ground state.

Jump frequency:

$$\Gamma_D = \nu Z \exp\left(-\frac{Q_D}{k_B T}\right) = \frac{2dD}{\lambda^2}$$

ν = atom vibration frequency ; Z nearest neighbors ; d = dimensionality

Phenomenological description of macroscopic diffusion

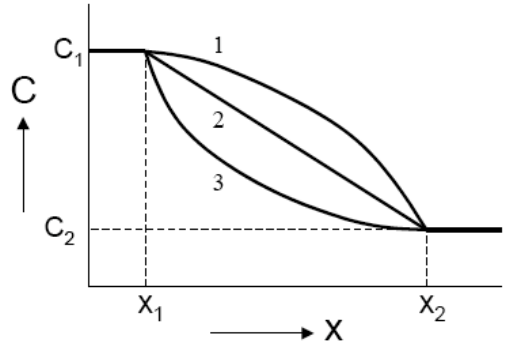
Flow of vacancies follows existence of gradients in concentration of vacancies (Fick's 1st law)
Prevails in steady states

Diffusion coefficient

$$J = -D\nabla n$$

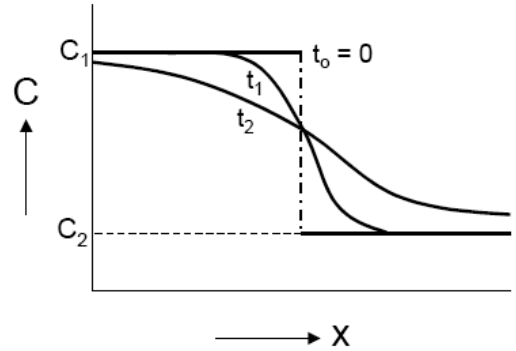
Flux
(# of vacancies crossing a unit area)

Concentration



Conservation of "mass" (Fick's 2nd law)
When composition changes with time

$$\frac{\partial n}{\partial t} = \nabla\left(D\nabla n\right)$$



Diffusion coefficient depends strongly on temperature

$$D = D_0 \exp\left(-\frac{Q}{kT}\right)$$

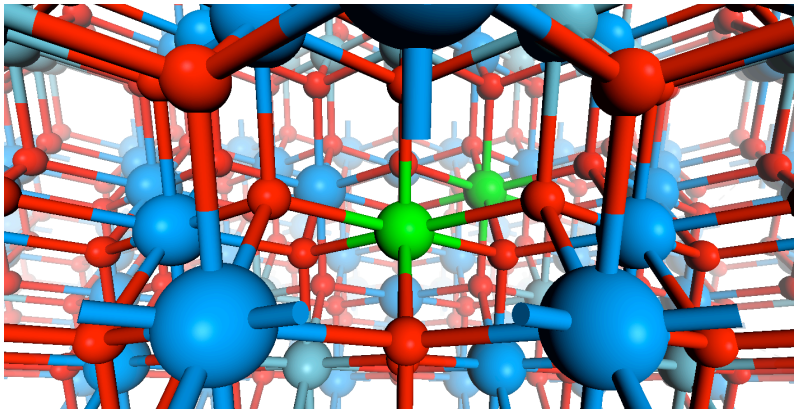
Activation energy for diffusion

MPALE: treat vacancy transport as continuum variable
Issue: dependence of D on strain gradient????

Ab Initio Investigation of Fission Product Gas Formation
(just starting)

Motivation:

- Meso-scale analysis of impact of fission product gas evolution on transient response of fuels possible with MPALE
- MPALE needs to be informed by lower length scale models (upscaling)
- Character of bubble formation and evolution strongly dependent on alloying
- Need ab initio methodology that can estimate the following in uranium alloys:
  - Bulk diffusivity of fission product gases
  - Equilibrium bubble sizes
  - Bubble diffusivity



U - blue, O - red, Kr - green

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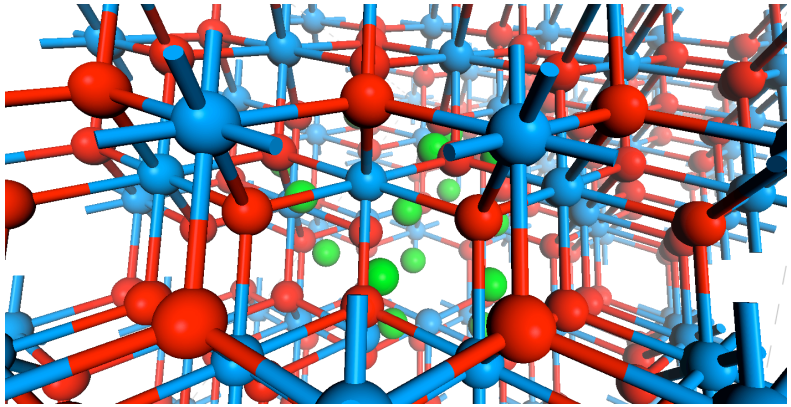
DFT for Bubble Formation

- **Method**
  - DMOL/VASP codes will be used
  - Tailored exchange-correlation energy functionals (A. Mattsson, SNL)
  - Collaboration (J. Wills, LANL) for extensions to heavier actinides



- **Steps**
  - UO_2 with isolated Kr impurities
    - Solution energy and atomic diffusivity, adjacent U sites (verification)
    - Solution energy for trapping Kr at defect sites (verification)
  - Extend to consider Kr-Kr interactions
    - Estimate equilibrium between Kr-Kr attraction and elastic distortion of U lattice
    - bubble size estimated
  - Extend study to Mixed Oxide (MOX) fuels

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Plasticity Validation - MPM

- **requirements**
  - small deformations
  - polycrystalline plasticity
  - implicit time integration

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Plasticity in MPM

J2 flow model:

$$\Phi(\boldsymbol{\tau}, q) := \| \operatorname{dev} \boldsymbol{\tau} \| - \sqrt{\frac{2}{3}}(\sigma_Y - q),$$

Small deformation ?!, NO microstructural details

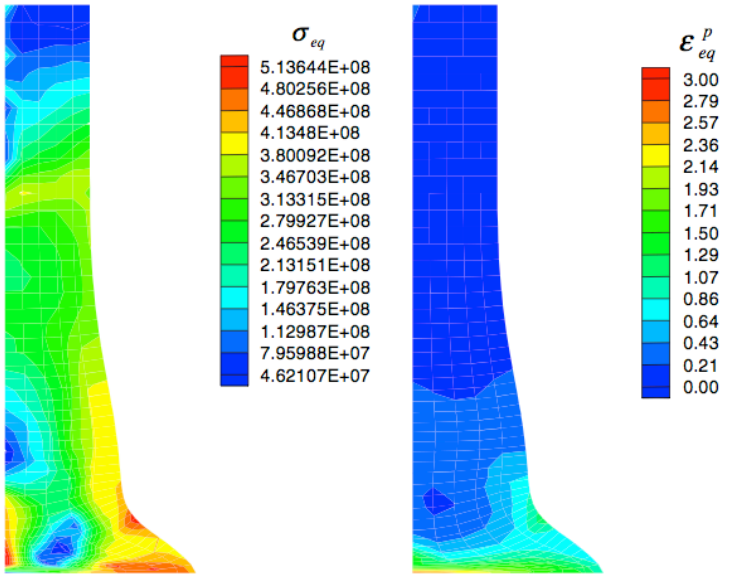
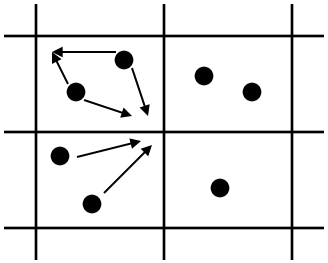


Fig. 6. Equivalent stress and plastic strain contours for bar impact.

Gadala,Comput. Methods Appl. Mech. Engrg. 193 (2004)

Deformation gradient in MPM

Mapping operations from particles to grid

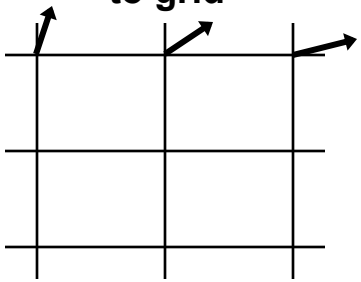


$$(m\mathbf{v})_i^t = \sum_{p=1}^{K} (M\mathbf{v})_p^t N_i(\mathbf{x}_p^t)$$

$$\mathbf{f}_i^{\text{int},t} = -\sum_{p=1}^{K} G_i(\mathbf{x}_p^t) \cdot \sigma_p^t \frac{M_p}{\rho_p^t}$$

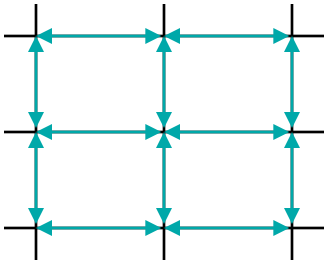
$$m_i^t = \sum_{p=1}^{K} M_p N_i(\mathbf{x}_p^t)$$

Apply boundary conditions to grid



$$\mathbf{f}_i^t = \mathbf{f}_i^{\text{int},t} + \mathbf{f}_i^{ext,t}$$

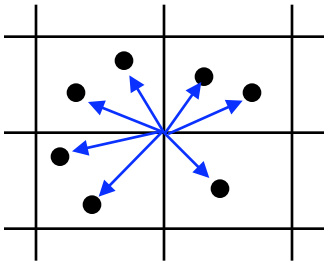
Update momentum at the grid



$$(m\mathbf{v})_i^{t+\Delta t} = (m\mathbf{v})_i^t + \mathbf{f}_i^t \Delta t$$

nodal forces + nodal momentum

Mapping operations from grid to particle

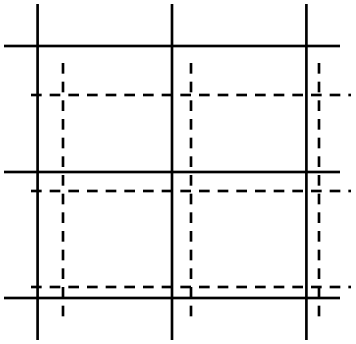


$$\mathbf{a}_p^t = \sum_{i=1}^{N} N_i(\mathbf{x}_p^t) \frac{\mathbf{f}_i^t}{m_i^t}$$

$$\overline{\mathbf{v}}_p^{t+\Delta t} = \sum_{i=1}^{N} N_i(\mathbf{x}_p^t) \frac{(m\mathbf{v})_i^{t+\Delta t}}{m_i^t}$$

$$\mathbf{x}_p^{t+\Delta t} = \mathbf{x}_p^t + \overline{\mathbf{v}}_p^{t+\Delta t} \Delta t$$

Update nodal information



$$(m\mathbf{v})_i^{t+\Delta t} = \sum_{p=1}^{K} (M\mathbf{v})_p^{t+\Delta t} N_i(\mathbf{x}_p^t)$$

$$\mathbf{x}_i^{t+\Delta t} = \mathbf{x}_i^{\Delta t} + \mathbf{v}_i^{t+\Delta t} \Delta t$$

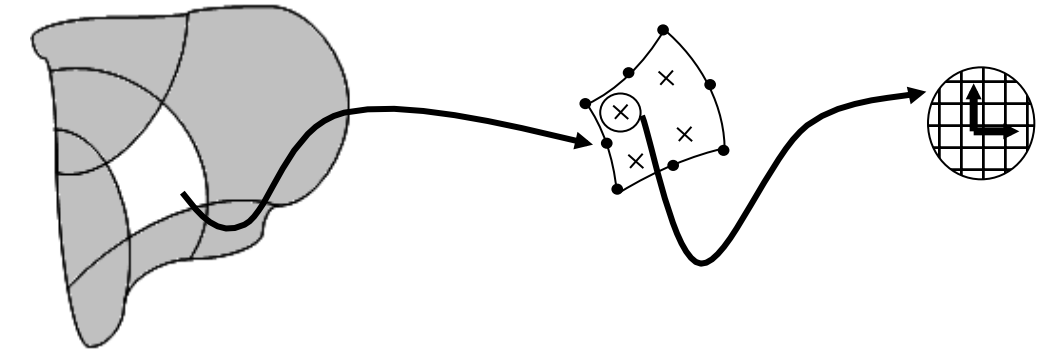
Update deformation gradient formulation

$$\mathbf{L}_p^{t+\Delta t} = \sum_{i=1}^{N} \mathbf{v}_i^{t+\Delta t} G_i(\mathbf{x}_p^t)$$

$$\mathbf{F}_p^{t+\Delta t} = \sum_{i=1}^{N} \mathbf{x}_i^{t+\Delta t} G_i(\mathbf{x}_p^t) \cdot \mathbf{F}_p^t$$

Crystal Plasticity Formulation

Microstructure captured by crystal plasticity



Single crystal

Finite Element

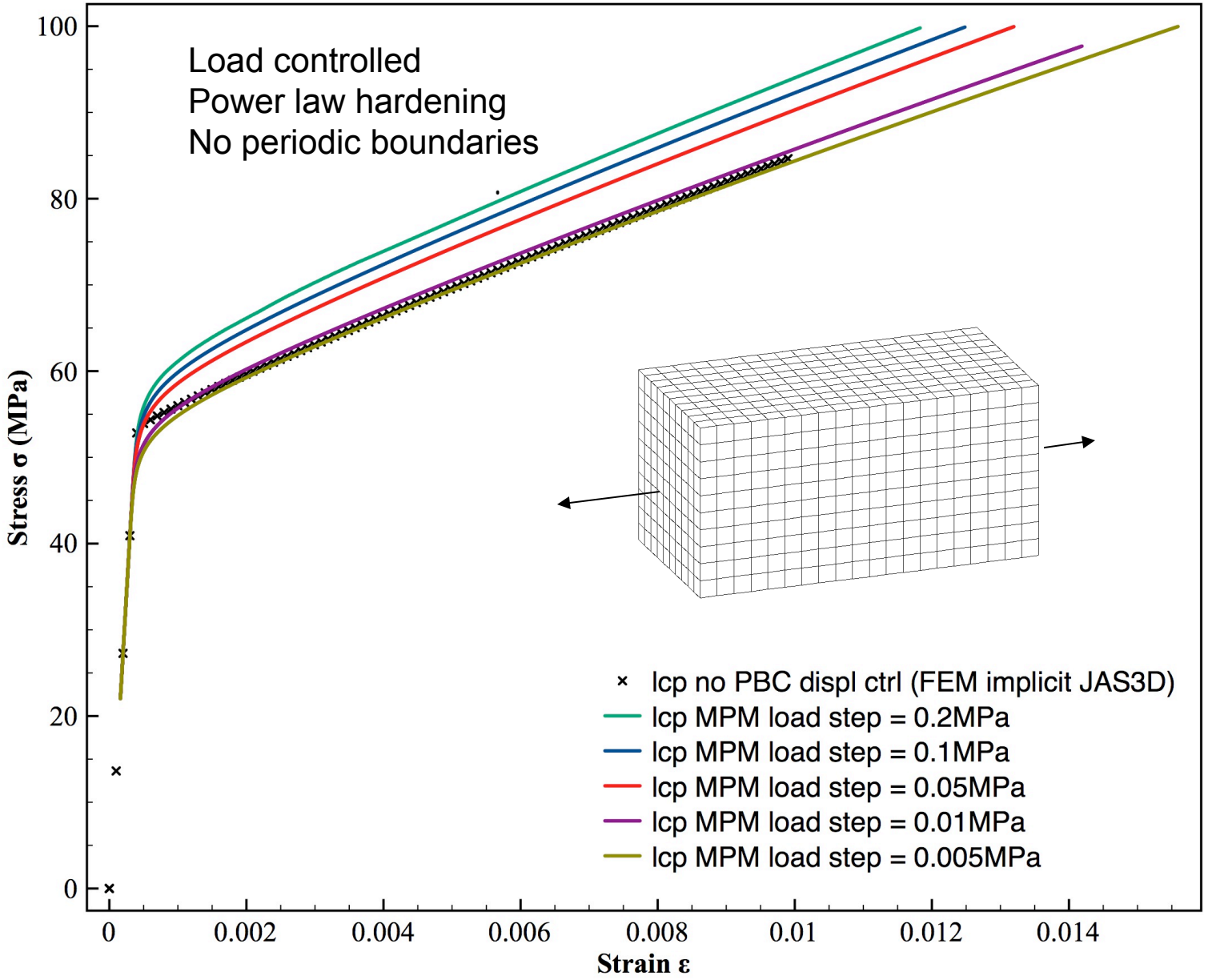
Particle-based

Slip Modes

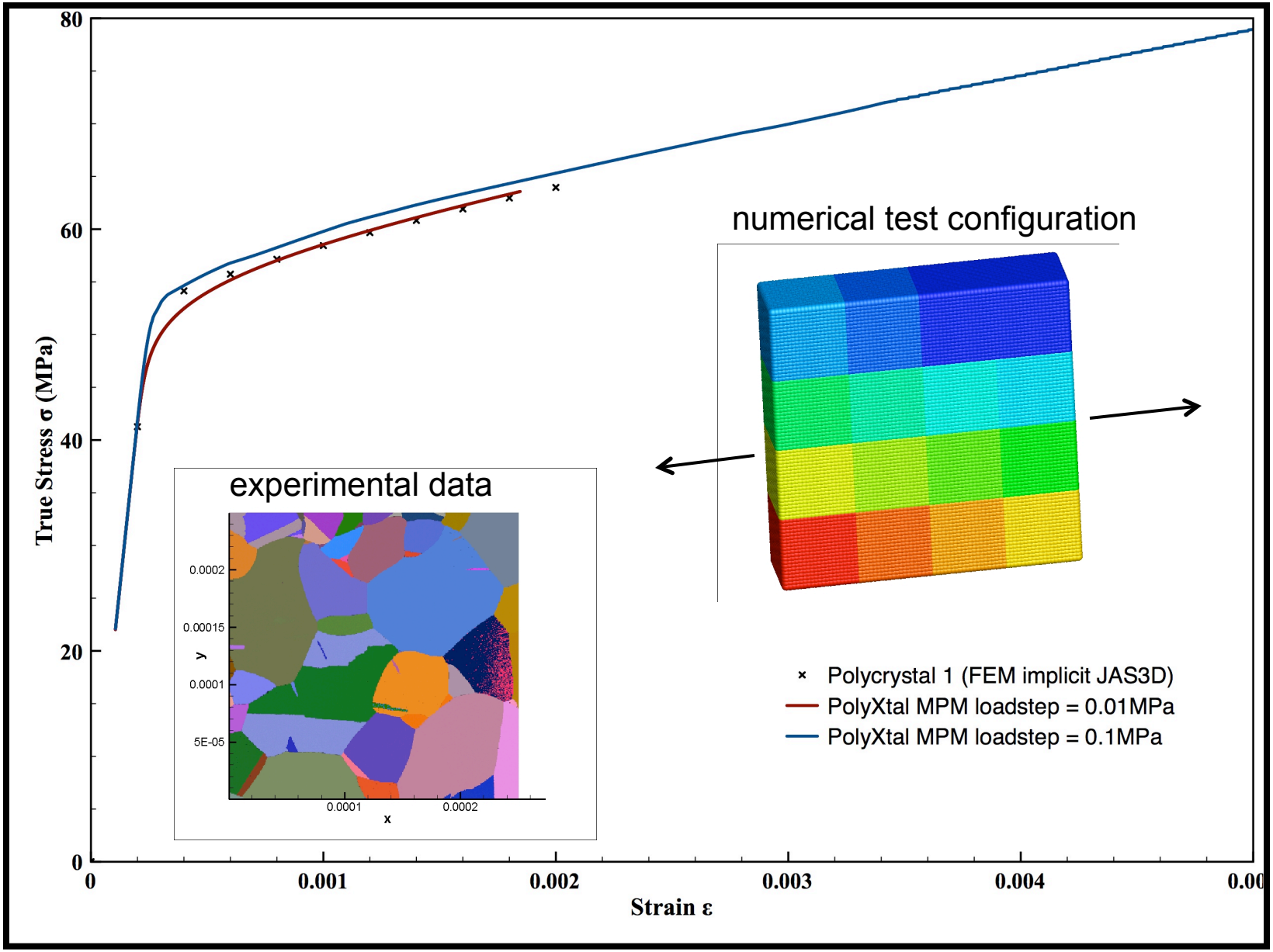
Balance laws

Constitutive Models

Comparison FEM (implicit) vs. MPM (explicit)
3D Single Crystal



Comparison FEM (implicit) vs. MPM (explicit)
3 D Polycrystal Crystal



Texture Evolution under Plastic Deformation

- **requirements**
  - coupled CMC and MPM
  - polycrystalline plasticity
  - implicit time integration

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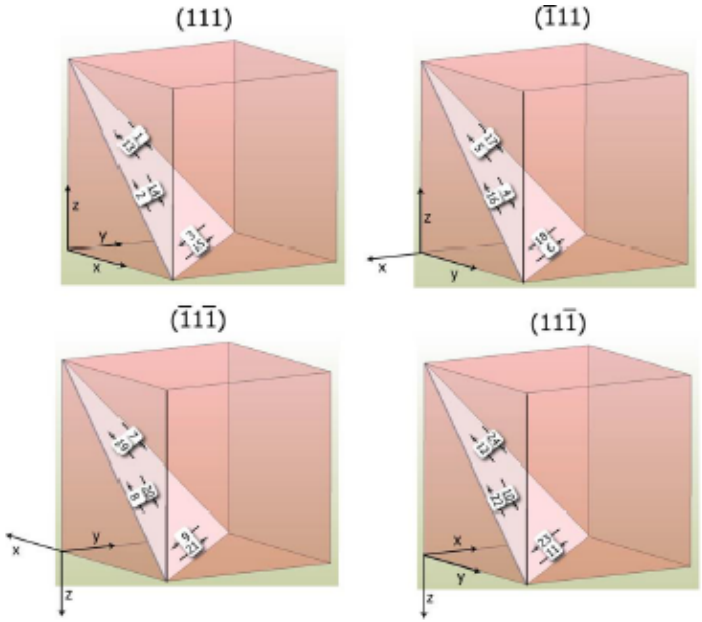
Constitutive Model

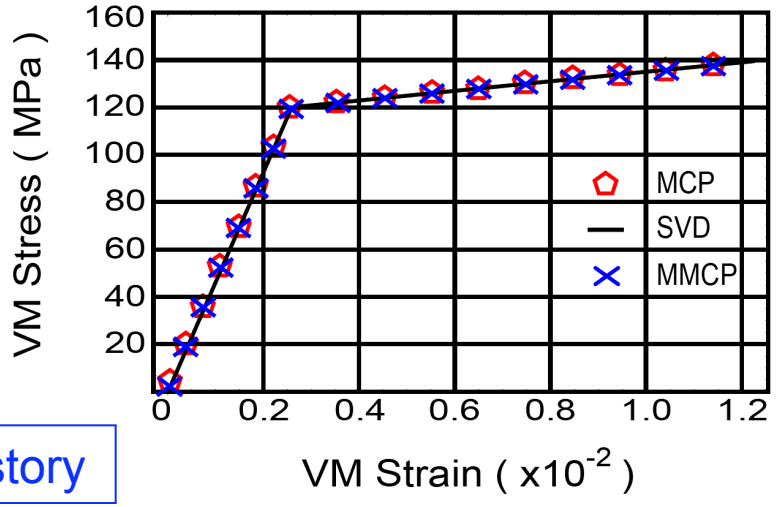
Elasticity

- General Hooke's law

Plasticity

- Traditional deterministic algorithm
  - Singular value decomposition & diagonal shift
  - Multiple activated slip systems
  - Limitations: high cost and possible redundant
- Monte Carlo plasticity model (MCP)
  - Probabilistic algorithm
  - One activated slip system
  - Limitations: small strain increment required
- Modified MCP
  - Multiple activated slip systems
  - Slip distributed by partition function
  - Limitations: small strain increment required





each MPM particle has its own slip plane history

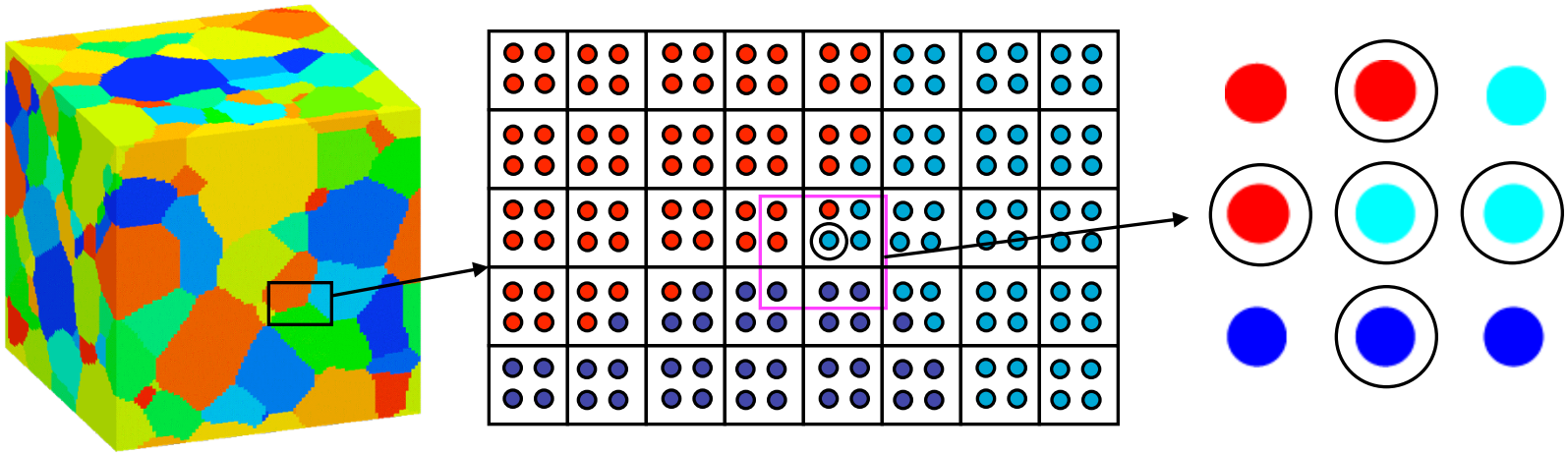
Kinetics: Metropolis Algorithm

- **MPM particles used for computing crystallographic orientation**
- **Probability of realizing a fluctuation event based on free energy reduction**
- **3 types of driving forces**
  - grain boundary energy, elastic energy, dislocation energy

$$\Delta G = \Delta E_s + \Delta E_m + \Delta E_b$$

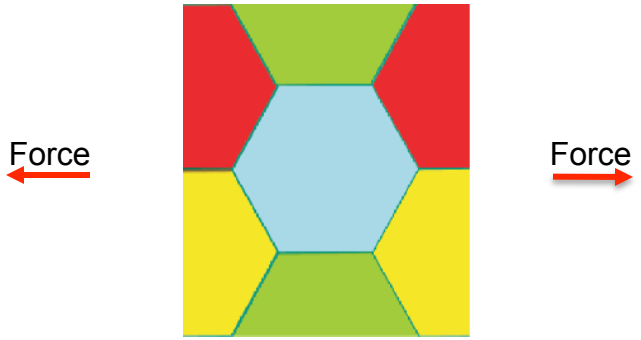
- **Particles tracked by Metropolis algorithm (Potts model)**

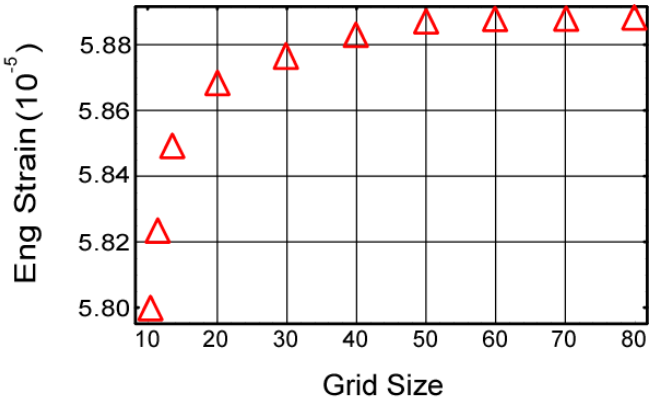
$$P(\Delta G) = \begin{cases} \exp(-\frac{\Delta G}{T}) & , \ \Delta G > 0 \\ 1 & , \ \Delta G \leq 0 \end{cases}$$

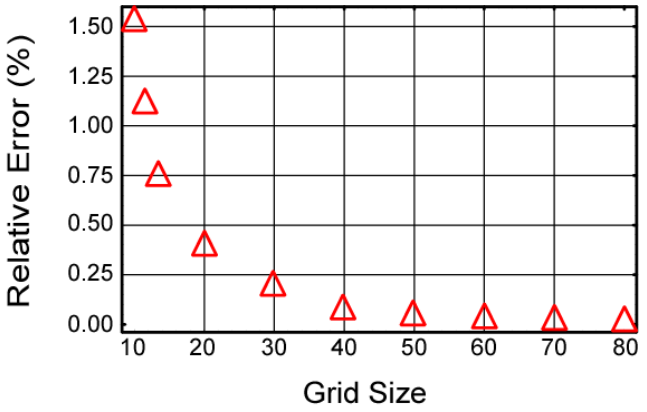


Numerical Errors: Mechanical, Polycrystal

- Domain:
  - Nickel polycrystal with 7 grains
- Setting:
  - Elastic deformation in 2D
  - Uni-axial loading
- Model:
  - MCP constitutive mode
- Convergence criterion
  - Relative stress increment
  - Strain increment
- Variation in total number of particles
  - PPC = 4
  - Domain size: Nx(4N/5)
- Conclusion
  - Need 12x10 domain for e <1%
  - 900 particles suggested for 3D grain







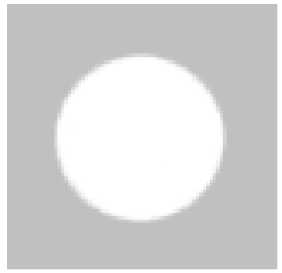
Numerical Errors: MC Simulation

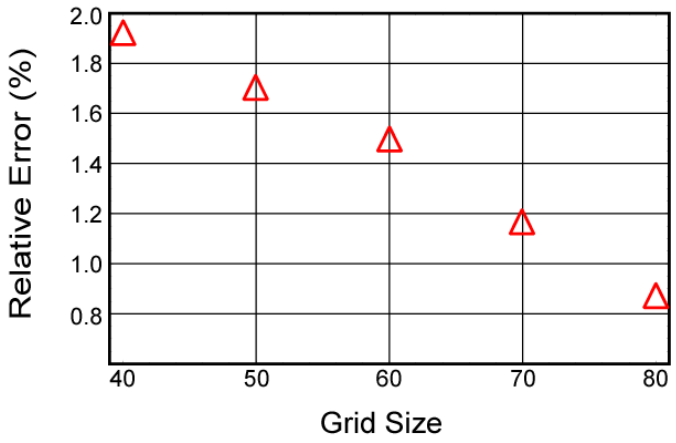
- Domain:
  - 3-D cube
- Setting
  - Spherical inner grain
  - Inner grain shrinks due to capillarity
- Model:
  - Two-state Ising
  - RB algorithm

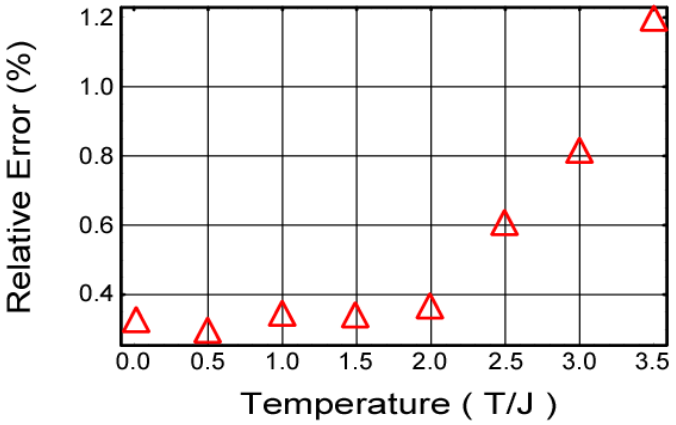
- Analysis:
  - Shrinking rate measured

- Variation in Domain Size
  - Temperature fixed: T/J=2.6
  - Domain size: 40^3 - 80^3
  - Relative errors decrease with grid size
  - Bigger domain suggested

- Variation in Fundamental Temperature
  - Domain size fixed: 60^3
  - Temperature range: T/J = 0 - 3.5
  - Relative error increases with temperature
  - Lower temperature suggested



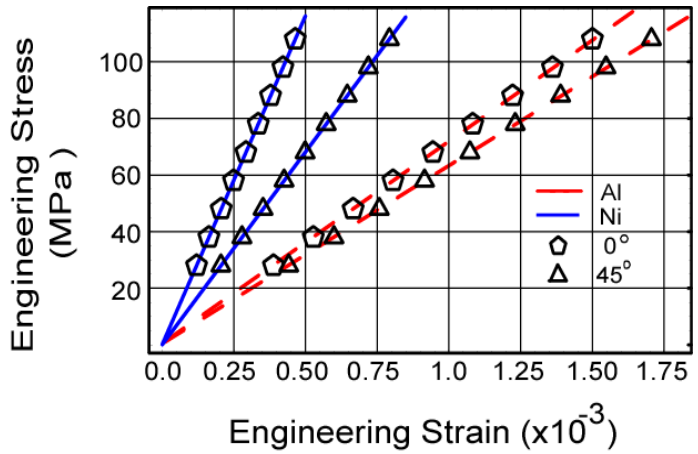




Experimental Accuracy: Elasticity

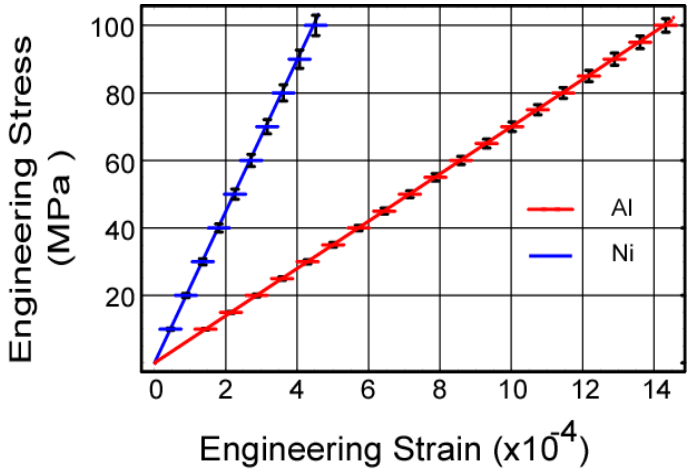
Single crystal

- Material: nickel, aluminum
- Domain size: 40^3 with 4 PPC
- Uni-axial loading
- Computed stress-strain relation
- Relative errors negligible
  - Homogeneous media (~0.15%)
  - Domain size effect small (~0.15%)



Polycrystal

- Material: nickel, aluminum
- Domain size: 60^3 with 4 PPC
- Uni-axial loading
- Computed stress-strain relation
- Error bars drawn
  - Aluminum microstructure effect (~2.0%)
  - Nickel microstructure effect (~3.0%)
  - Domain size effect (~0.15%)

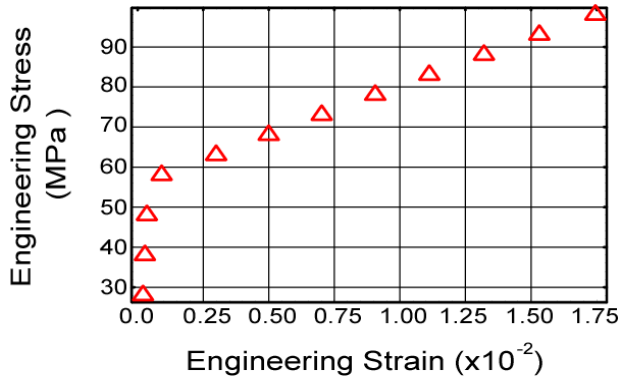


Expt. Data Source: M. Nygards, Mech of mater. 35 (2003).

Experimental Accuracy: Plasticity

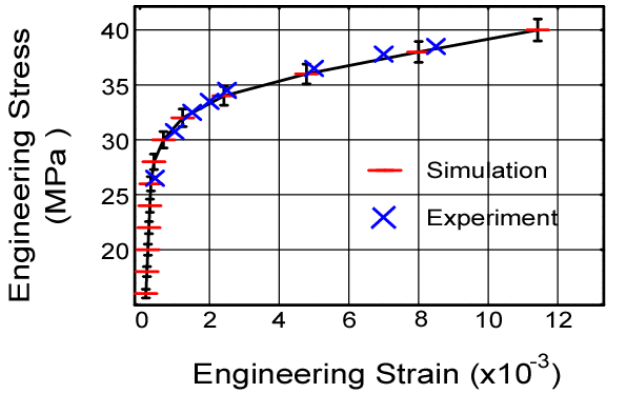
Single Crystal

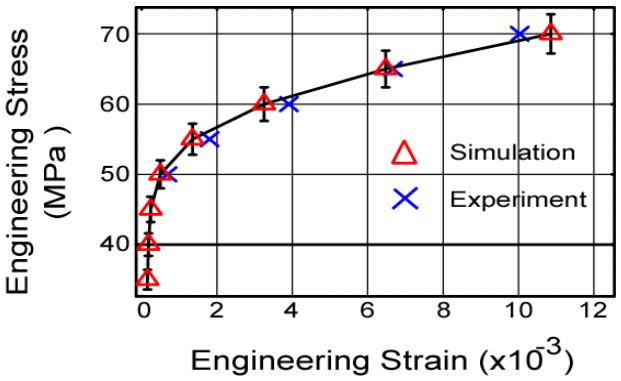
- Domain size: 40^3 with 4 PPC
- Nickel
- Uni-axial loading
- Relative errors negligible
  - Homogeneous media (~0.15%)
  - Domain size effect is small (~0.15%)



Polycrystal

- Domain size: 60^3 with 4 PPC
- Nickel and aluminum
- Uni-axial loading
- Constitutive model: MCP with T/J = 1.0
- Computed stress-strain relation
- Error bars drawn
  - Aluminum microstructure effect (~2.0%)
  - Nickel microstructure effect (~3.0%)
  - Domain size effect (~0.5%)
  - Temperature effect (~0.5%)
- No size effect captured due to the local plasticity model (MCP) implemented





Expt. Data Sources:

B. Clausen, Metallurgical and Materials Transactions A. 28 (1997).

W. Counts, Ph.D. thesis. (2007).

MC Calibration in Subsequent Applications

MPM physical domain

- Nickel polycrystal
- Domain size: 1 mm cube
- MPM grid: 1 million particles with 64 ppc
- Uni-axial loading in the x-direction
- Grain boundary mobility: (~10^{-12} m^4/J-s)
- Grain boundary energy: (~0.45 J/m^2)

MC domain

- 1 million lattice sites
- Fundamental temperature: T/J = 2.6
- Reduced grain boundary mobility: 0.27

Time and length scale

- Characteristic length: 10 microns
- Characteristic time: $t_0 = \frac{M^* l_0^2}{M^*} = 60s$
- **1 MCS = 1 min, 1 MPL step ~ 1 ms**

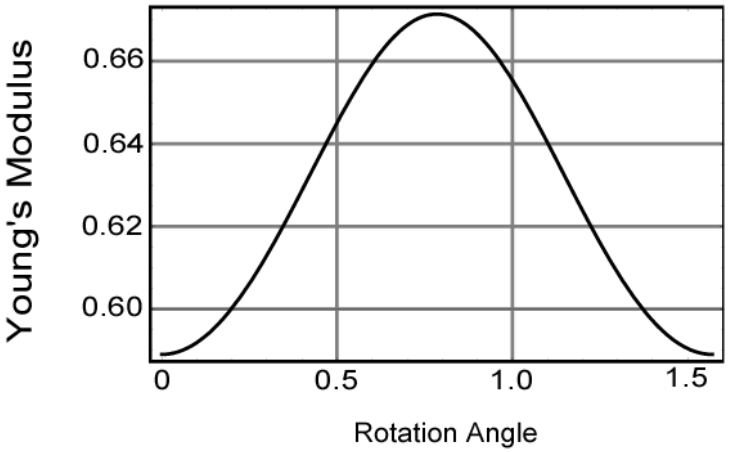
F. Humphreys, Recrystallization and related annealing phenomena (2004).

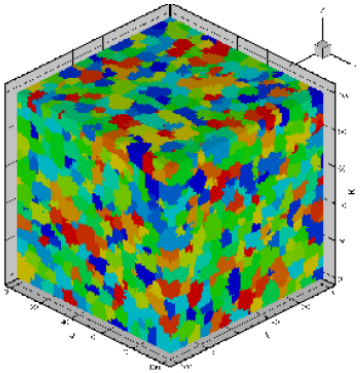
Texture Evolution: Application 2

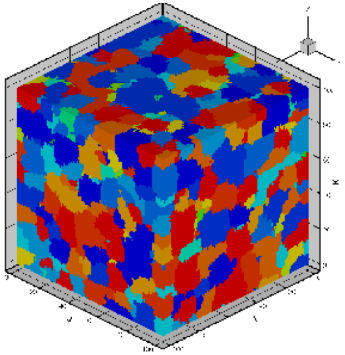
Texture evolution driven by elastic loading

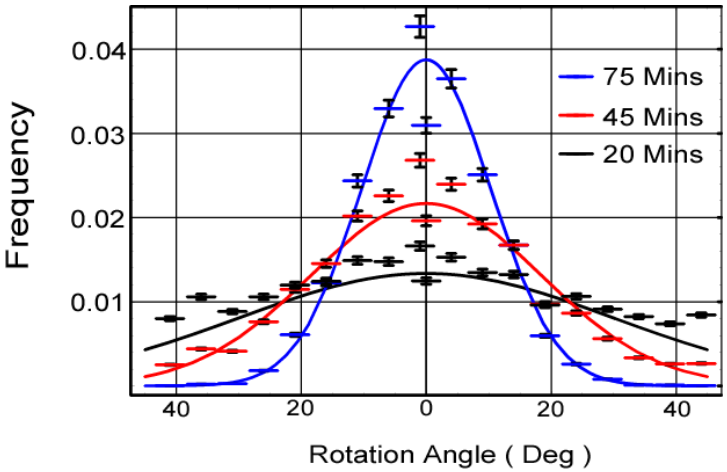
- Domain size: 100^3 with 4 PPC
- Physical domain size: 1 mm in each dimension
- Initial configuration: 91 orientations (random)
- Uni-axial loading: 30 MPa
- Fundamental temperature: T/J=2.6
- Physical temperature: T= ~600 k
- Driving force: grain boundary & elastic energy
- Error bars drawn
  - Microstructure effect (~1.5%)
  - Domain size effect (~0.5%)
  - Temperature effect (~0.7%)

- Softer materials (wrt loading direction) survive







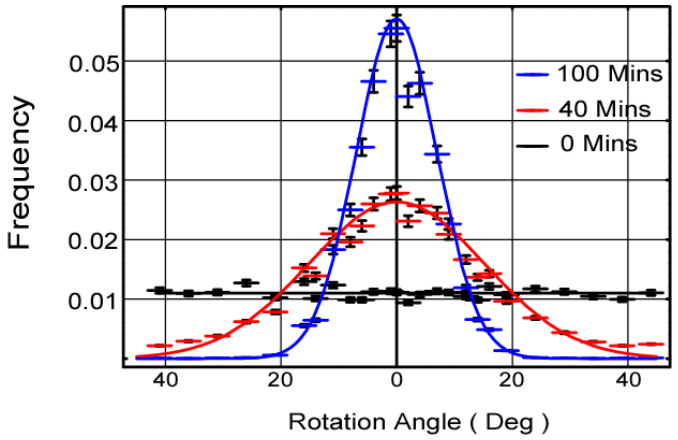


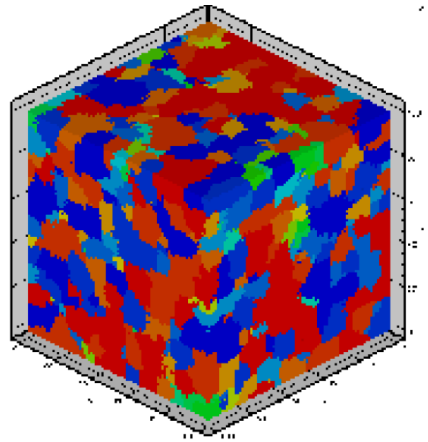
Texture Evolution: Application 4

Texture evolution driven by elastic and plastic loading

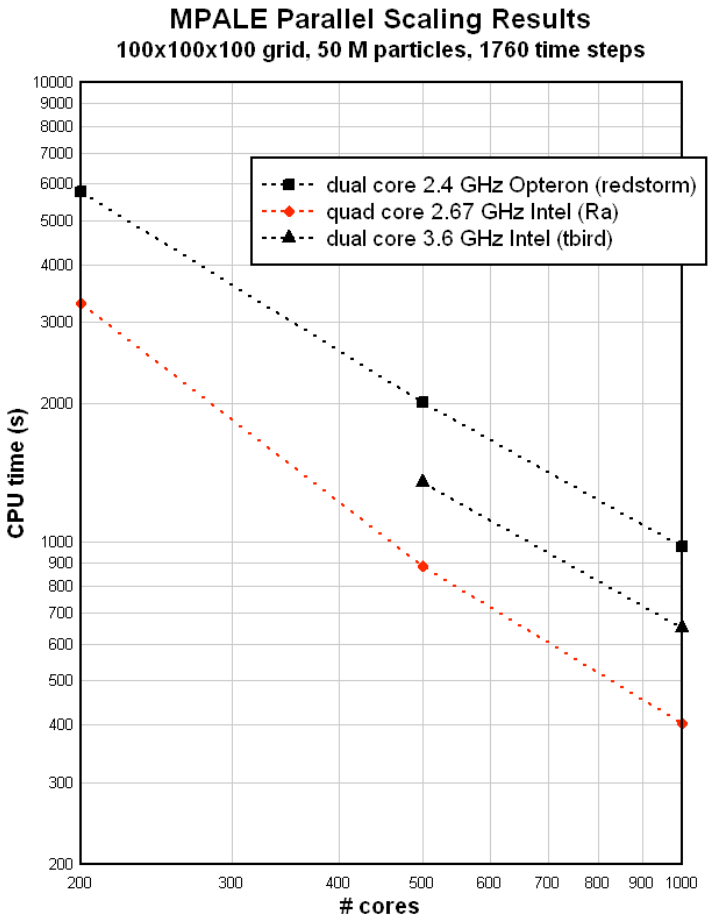
- Domain size: 100^3 with 4 PPC
- Physical domain size: 1 mm in each dimension
- Initial configuration: 91 orientations (random)
- Uni-axial loading: 20 MPa
- CRSS : 8 MPa
- Fundamental temperature: T/J = 2.6
- Physical temperature: T = ~600 k
- Driving force: grain boundary, elastic and dislocation energy
- Error bars drawn
  - Microstructure effect (~1.5%)
  - Domain size effect (~0.5%)
  - Temperature effect (~0.7%)

- Materials with smaller Schmid factors and Young's modulus (wrt loading direction) survive





Parallel Computational Efficiency of MPALE



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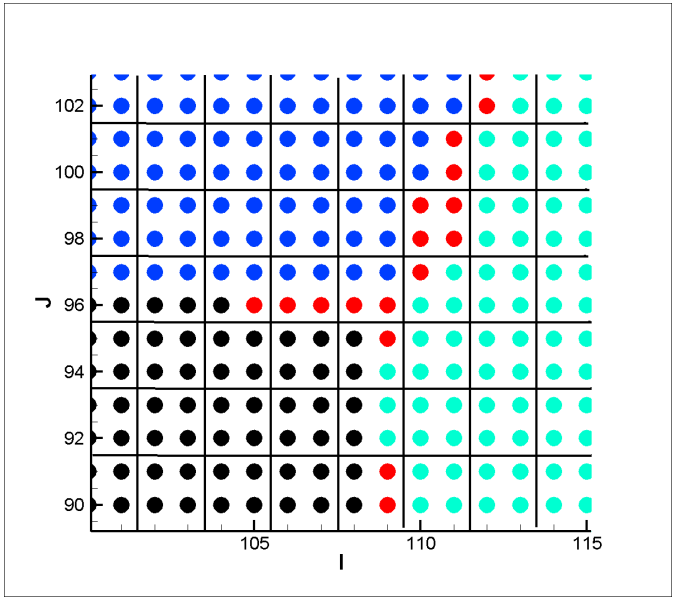
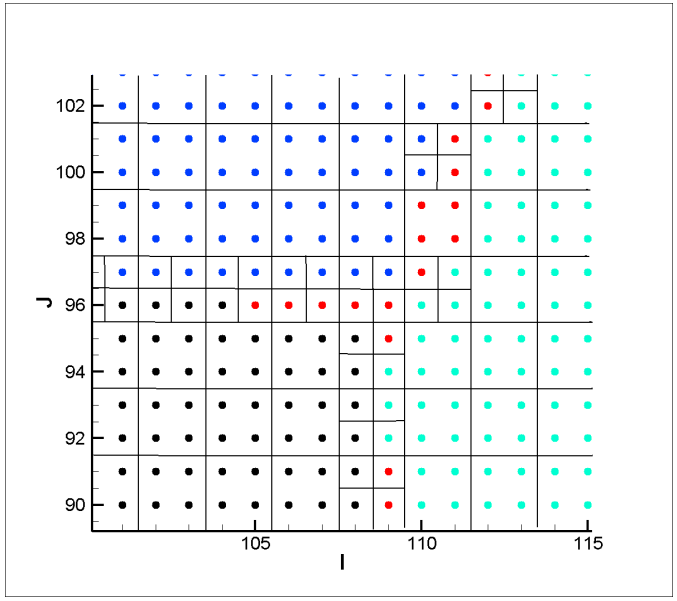
Summary

- **Particle & cell characteristics of MPM useful for multiple length scale coupling**
- **successful MPM validation for fuel pin problem**

- **discussion topics:**
  - MPM vs single point FEM grids
    - – multi-material interface issues
  - automatic multi-grid (similar to Fehlberg R-K?)





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Framework of crystal plasticity

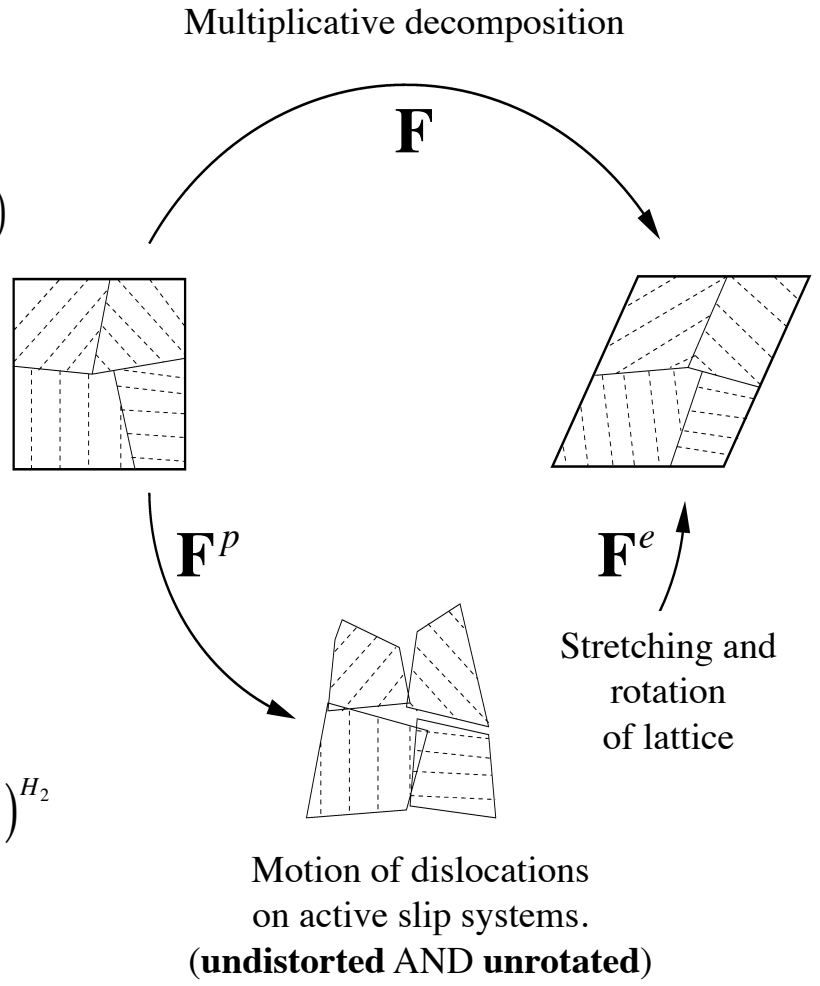
Elasticity $\sigma^{PK2} = \mathbf{C}^e : \tilde{\mathbf{E}}^e$

Kinematics of slip systems $\mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1} = \sum_{\alpha=1}^{Nslip} \dot{\gamma}^a \left(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \right)$

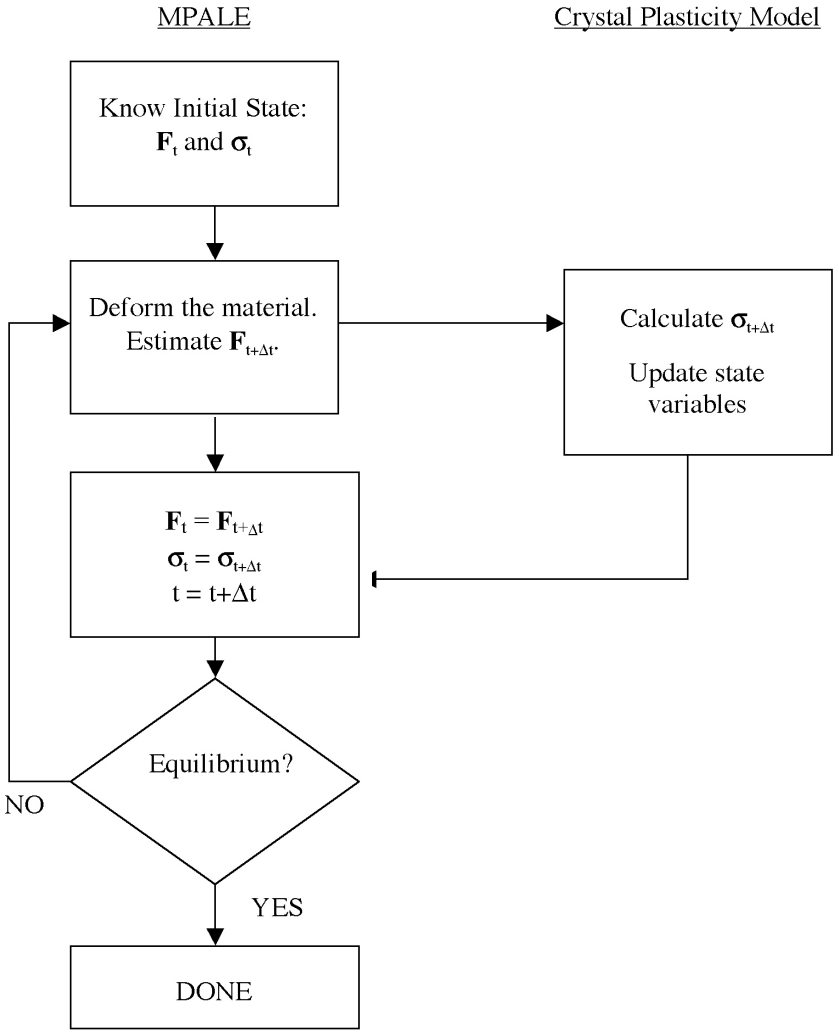
Crystallographic slip
=
Dominant plastic deformation mechanism

Slip system evolution
(power law viscoplastic flow rule) $\dot{\gamma} = \dot{\gamma}_0 \left| \frac{\tau^a}{\tau^a_{CRSS}} \right|^{1/m} \mathrm{sgn}\left(\tau^a\right)$

Slip system hardening Power law $\tau^\alpha_{CRSS} = \tau_0 + H_1 \left(\varepsilon^p\right)^{H_2}$



Crystal plasticity in MPM



$$\tau_t^\alpha = \sigma_t : (s^\alpha \otimes m^\alpha)$$

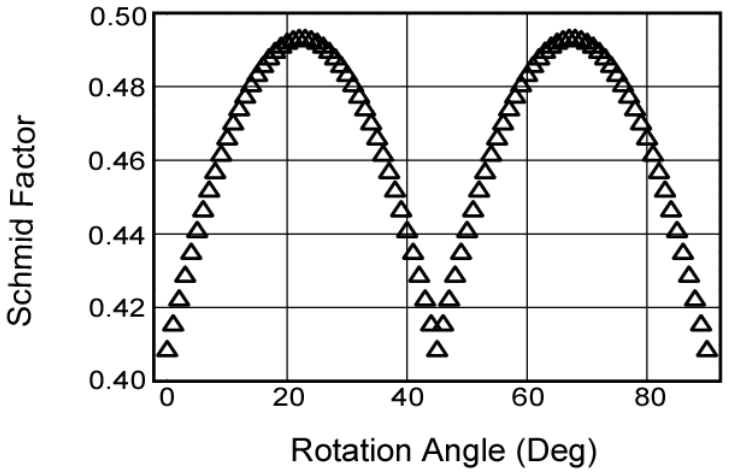
$$\dot{\gamma}_t^\alpha = \gamma_0 \left| \frac{\tau_t^\alpha}{\tau_t^{CSS-\alpha}} \right|^{\frac{1}{m}} \operatorname{sgn}\left(\tau_t^\alpha\right)$$

Update: $\sigma_{t+\Delta t}$ and $\tau_{t+\Delta t}^{CSS-\alpha}$

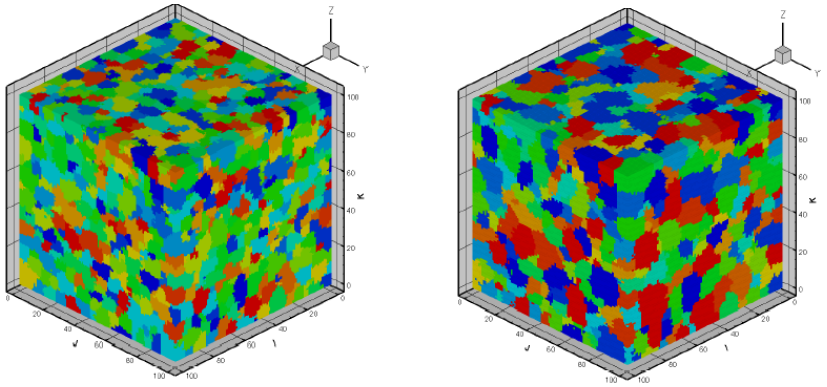
Texture Evolution: Application 3

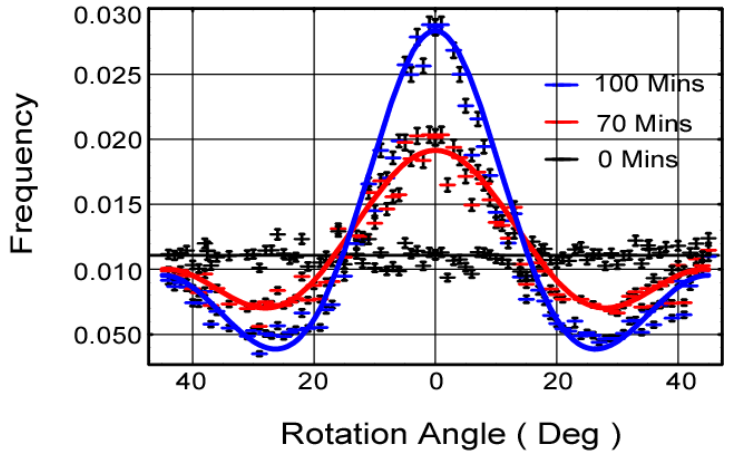
Texture evolution driven by plastic loading

- Domain size: 100^3 with 4 PPC
- Physical domain size: 1 mm in each dimension
- Initial configuration: 91 orientations (random)
- Uni-axial loading: 20 MPa
- CRSS : 8 MPa
- Fundamental temperature: T/J=2.6
- Physical temperature: T= ~600 k
- Driving force: grain boundary & dislocation energy
- Error bars drawn
  - Microstructure effect (~1.5%)
  - Domain size effect (~0.5%)
  - Temperature effect (~0.7%)



- Materials with smaller Schmid factors (wrt loading direction) survive



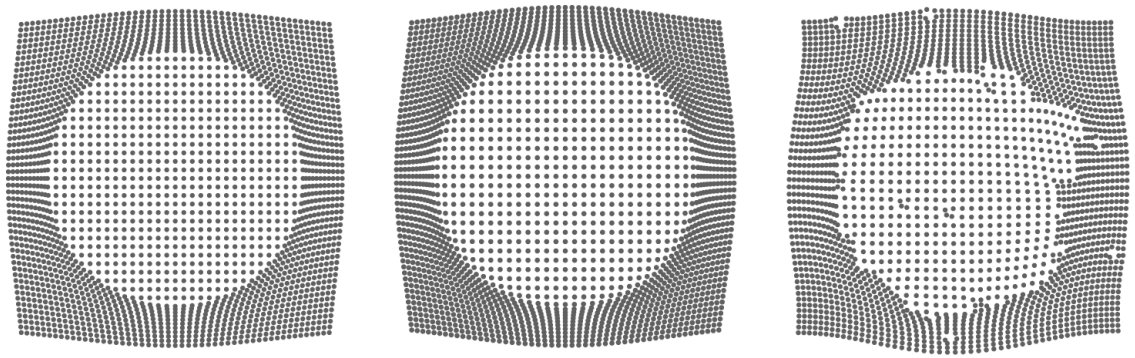


Hybrid Monte Carlo Method

- **Meso-scale Mechanics**
  - Mesh-based FEM and FDM
    - limitations: re-meshing and grain boundary tracking
  - Meshless MPM
    - simple grain boundary definition and tracking

- **Meso-scale Kinetics**
  - Phase-field and sharp-interface
    - demanding in 3D
  - Monte Carlo models
    - straightforward to implement in 3D

- **Current Work: Hybrid Monte Carlo**
  - Deterministic mechanics and probabilistic grain boundary kinetics



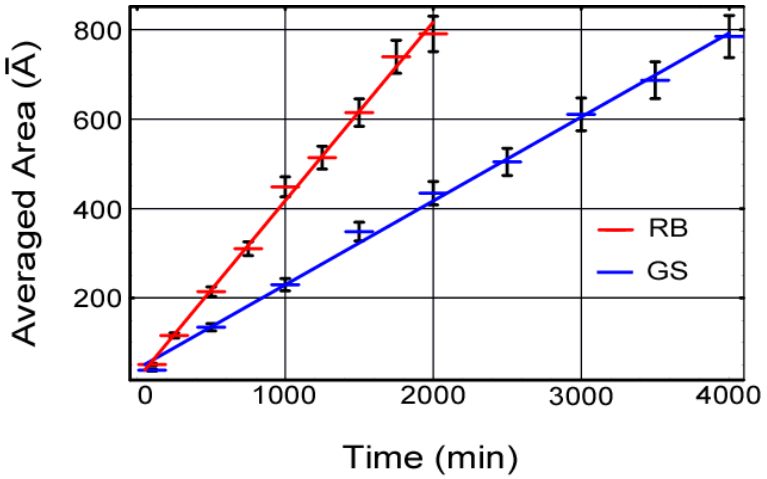
Experimental Accuracy: Kinetics

Isotropic grain growth theory and experiments

- Mean grain radius: $R = ct^{1/n}$, n = 2
- Mean grain area: $A = c_1 t$
- Mean grain volume: $V^{3/2} = c_2 t$

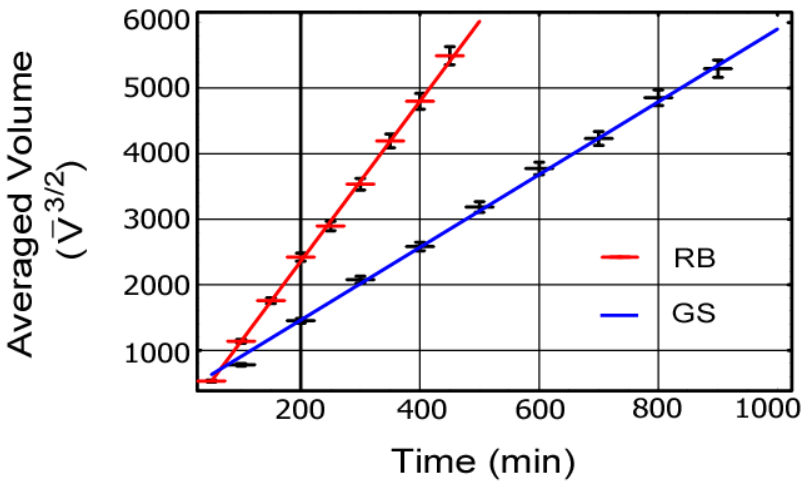
Isotropic grain growth in 2D

- Domain size: 200x200
- Isotropic grain boundary energy
- Temperature: T/J=1.0
- GS and RB updating rules
- Compared with experimental data
- Error bars drawn
  - Temperature effect (~2.5%)
  - Domain size effect (~2.5%)



Isotropic grain growth in 3D

- Domain size: 40 cube
- Isotropic grain boundary energy
- Temperature: T/J=1.0
- Gs and RB updating rules
- Error bars drawn
  - Temperature effect (~0.05%)
  - Domain size effect (~2.0%)



F. Humphreys, Recrystallization and related annealing phenomena (2004).