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Modeling the mechanical behavior of amorphous and crystalline engineering materials

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Computational Materials Science & Engineering, Sandia National Laboratories

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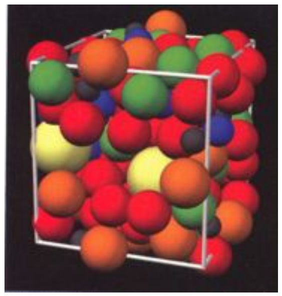
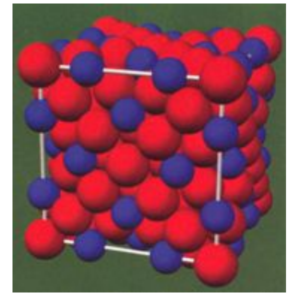
Amorphous vs. Crystalline


Liquidmetal Technologies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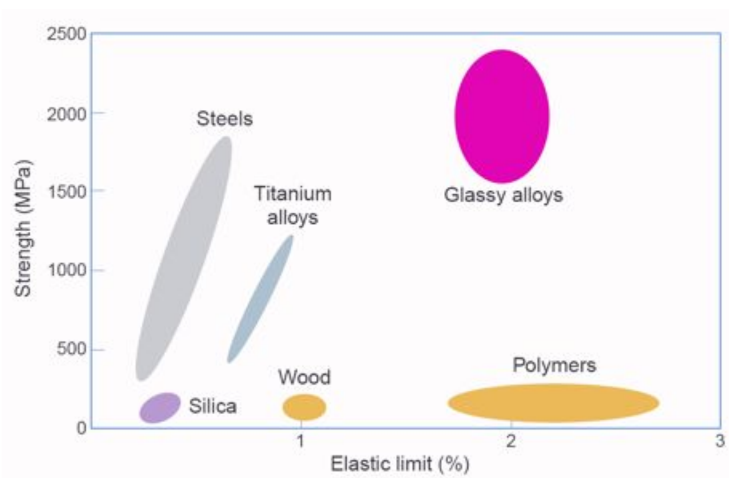
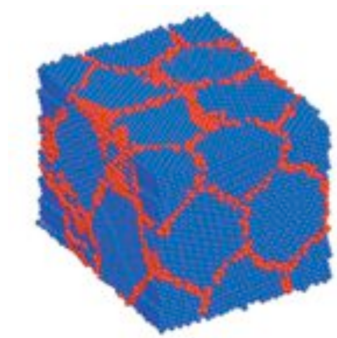
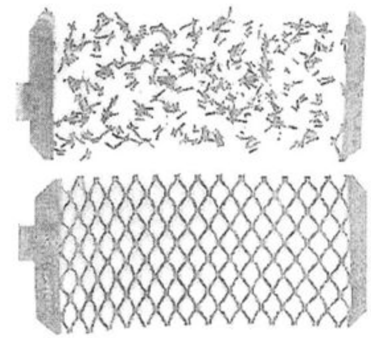
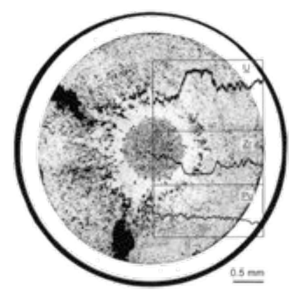


Telford. Materials Today 2004.


Schuh Group, MIT.

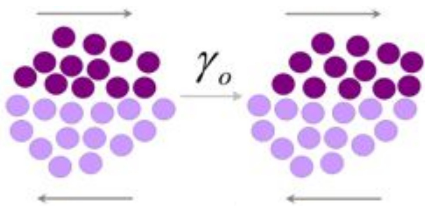

Palumbo, et al. JOM. 1998.


Kim, et al. J. Nucl. Mat. 2004.

Presentation Topics

Amorphous Metals

Development & Validation



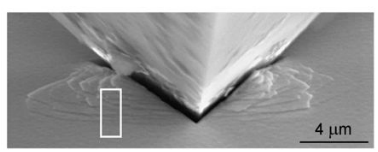
Kinetic Monte Carlo
Finite Element Analysis
2D & 3D

Applications

Shear Localization

Shi. Falk. Scr. Mat. 2006.

Nano-Indentation

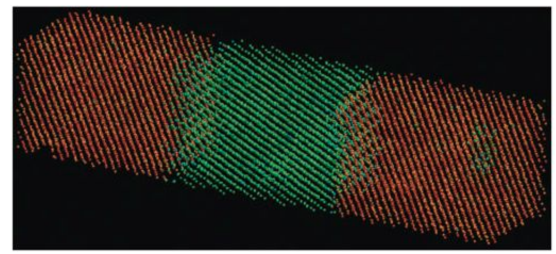


Moser, et al. Phil. Mag. 2006.

Polycrystalline Metals

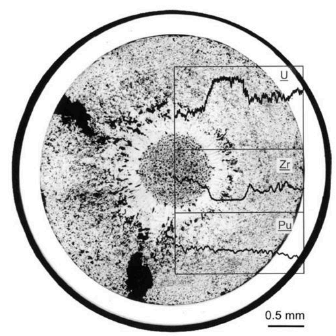
Grain Boundary Motion

Atomistic Simulations



Janssens, et al. Nat. Mat. 2006.

Microstructure Evolution



Potts Monte Carlo

Phase Field

Kim, et al. J. Nucl. Mat. 2004.

Presentation Topics

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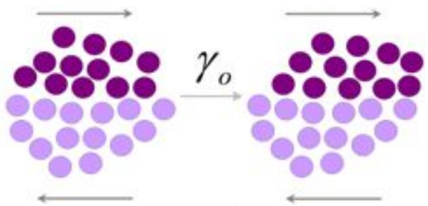
Development & Validation



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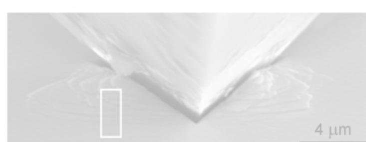

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Polycrystalline Metals

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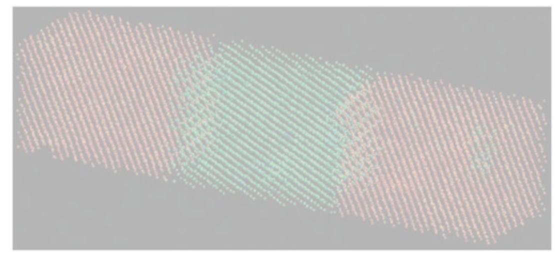

Janssens, et al. Nat. Mat. 2006.

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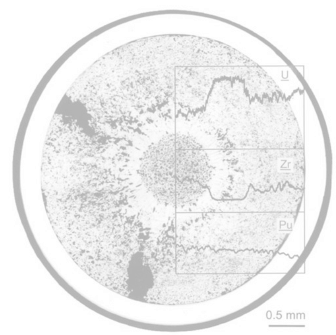

Potts Monte Carlo

Phase Field

Kim, et al. J. Nucl. Mat. 2004.

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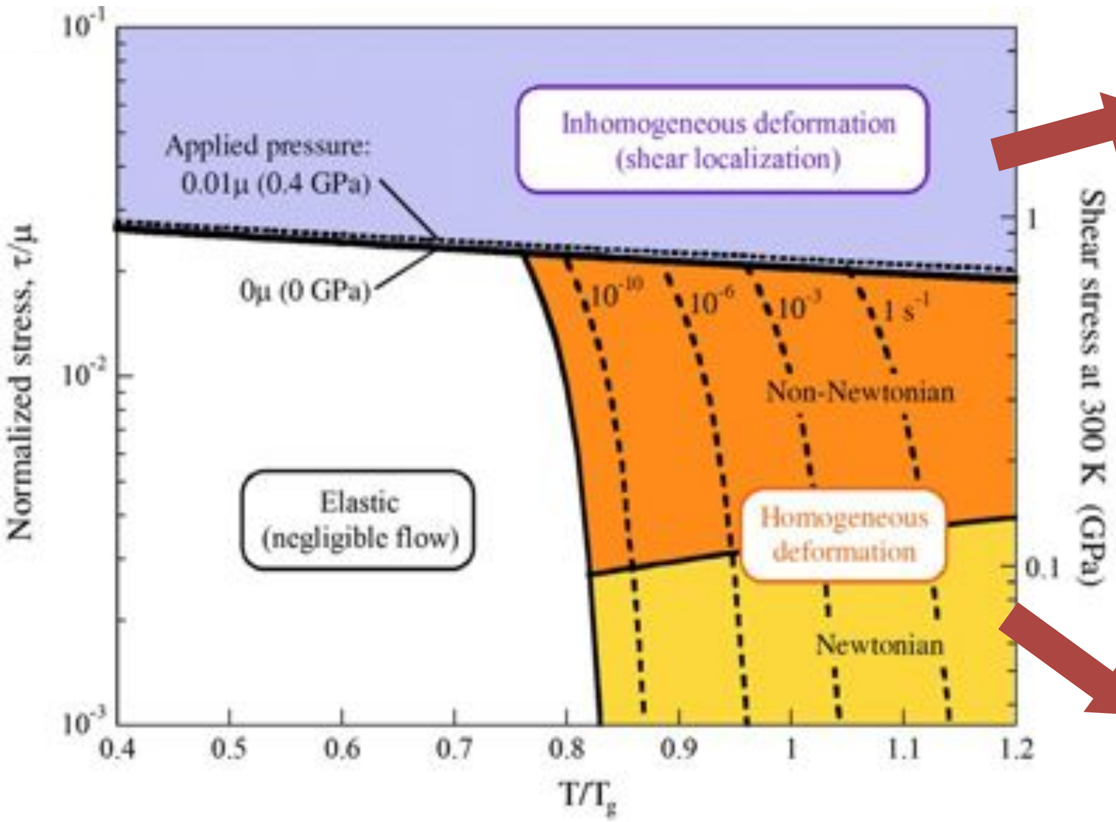
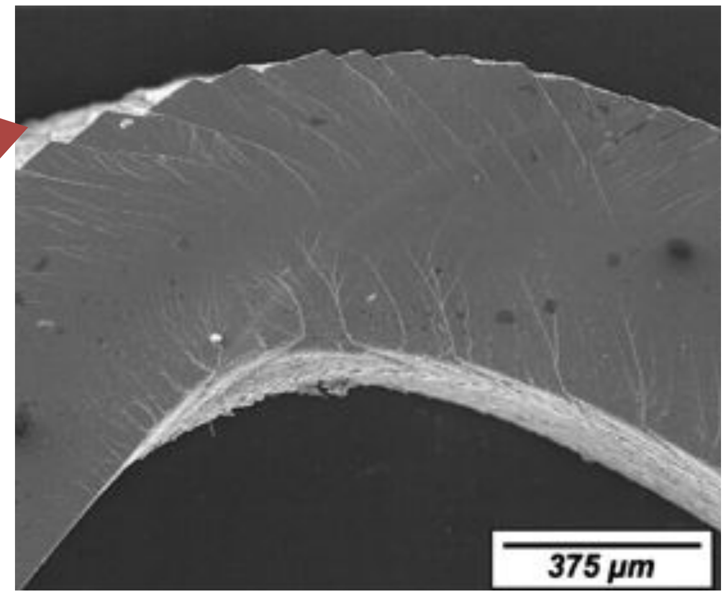
Mechanical behavior of an amorphous metal



Schuh et al. Acta Mat. 2007.

Shear Band Event
Propagation: 10^{-5}-10^{-3} s
Thickness: 10^{-8} m



Conner et al. J. Appl. Phys. 2003.

Kawamura et al. Scripta Mat. 1998.

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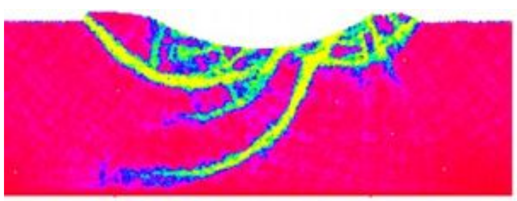
Combined approach of modeling techniques

Atomistic Simulations

- Interatomic Potentials
- Time Scale ~ $10^{-12} - 10^{-6}$
- Strain Rate ~ $10^{6} - 10^{8}$
- Length Scale ~ 10^{-9}

Continuum Simulations

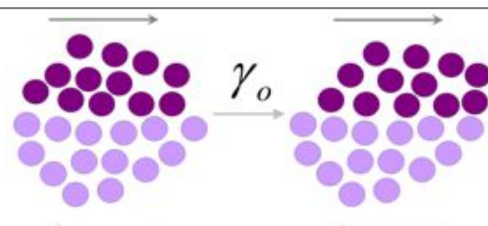
- Constitutive Relation
- Longer Time Scale
- Range of Strain Rates
- Larger Length Scale



Shi, Falk. Acta Mat 2007.

Meso-scale Simulations

- Characteristic Event, STZ
- Time Scale ~ $10^{-9} - 10^{-3}$
- Length Scale ~ $10^{-9} - 10^{-6}$



Argon. Acta Metall. 1979.

Su, Anand. Acta Mat 2006.

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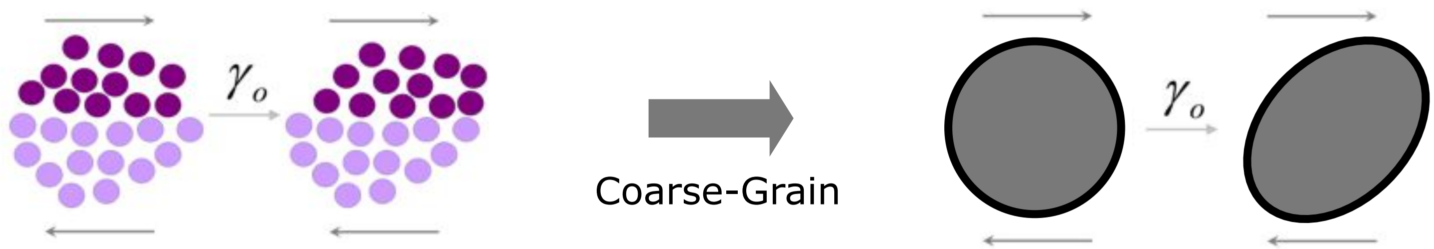
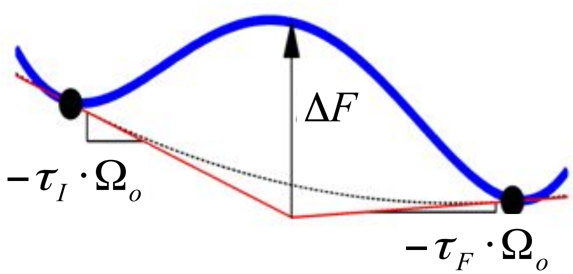
Coarse-graining the shear transformation zone



Argon. Acta Metall. 1979.

Potential Energy Landscape

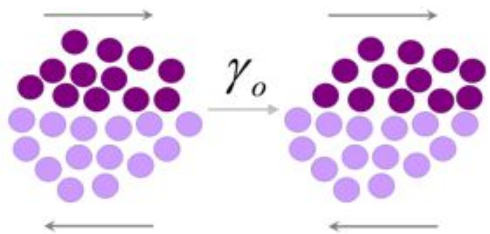
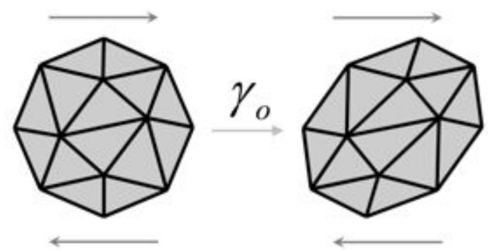
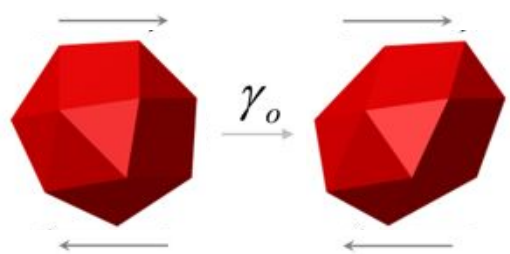


Bulatov, Argon. Model. Simul. Mater. Sci. Eng. 1994.

Characteristic Attempt Frequency

$$\dot{s} = \nu_o \cdot \exp\left(- \frac{\Delta F - \frac{1}{2}\tau \cdot \gamma_o \cdot \Omega_o}{kT} \right)$$

Key elements for a mesoscale model

	Coarse-Grain	STZ Activation Rate
STZ		$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F - \frac{1}{2}\tau \cdot \gamma_o \cdot \Omega_o}{kT}\right)$
2D		$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F}{kT}\right) I_o\left(\frac{\tau_{\max} \cdot \gamma_o \cdot \Omega_o}{2kT}\right)$
3D		$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F}{kT}\right) \iiint_{g \in G} \exp\left(-\frac{\tau(\sigma, g) \cdot \gamma_o \cdot \Omega_o}{2kT}\right) dg$

Numerical Accuracy: 2D error ~1%, 3D error ~2%

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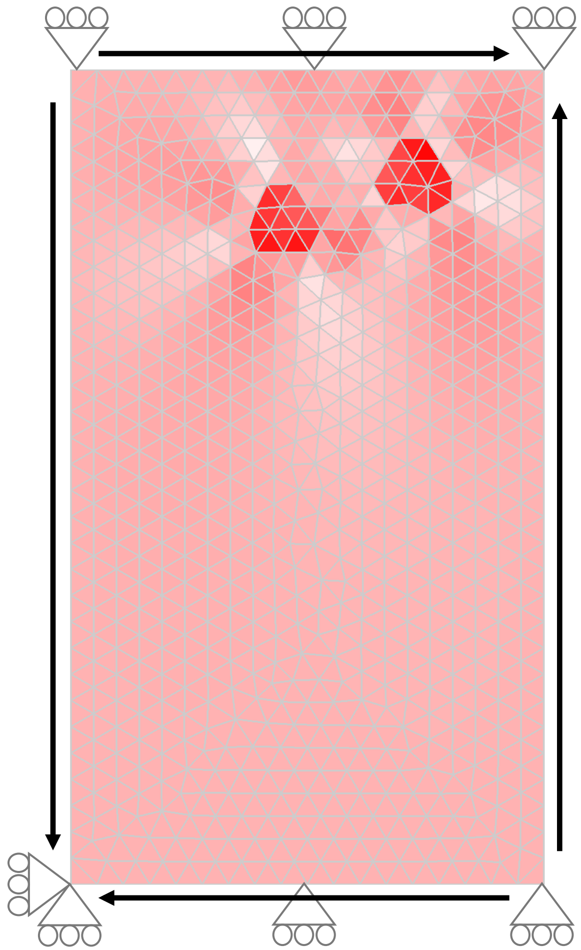
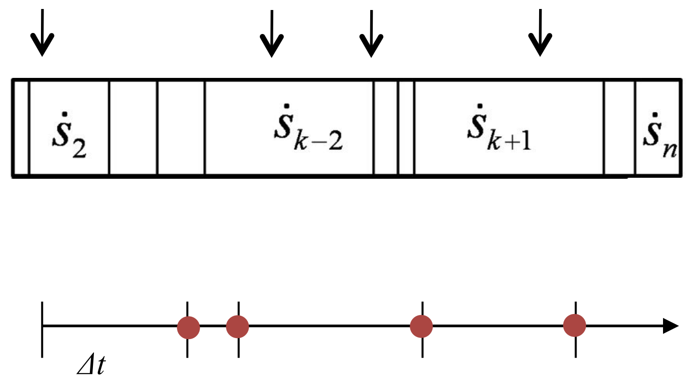
Kinetic Monte Carlo algorithm for STZs



Kinetic Monte Carlo

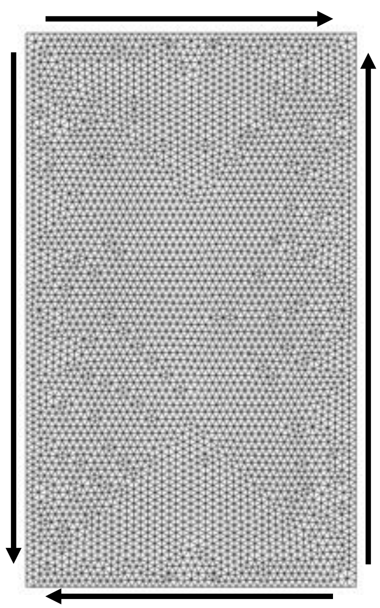
$$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F}{kT}\right) \iiint_{g \in G} \exp\left(-\frac{\tau(\sigma, g) \cdot \gamma_o \cdot \Omega_o}{2kT}\right) dg$$



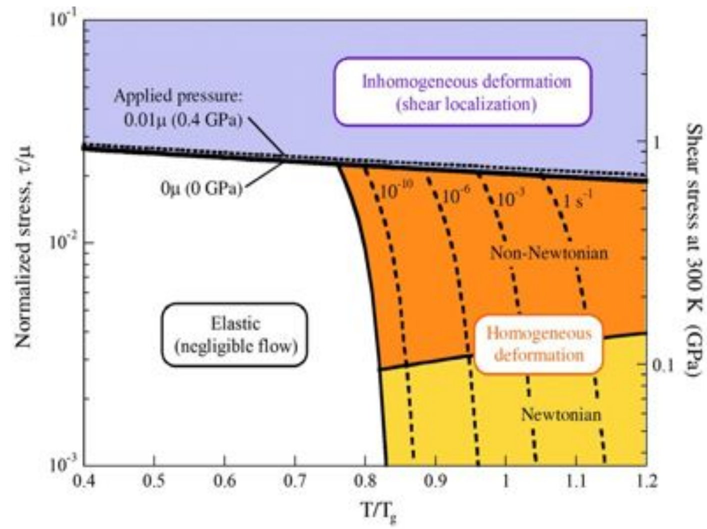
ABAQUS

Validation of the STZ Dynamics framework

2D



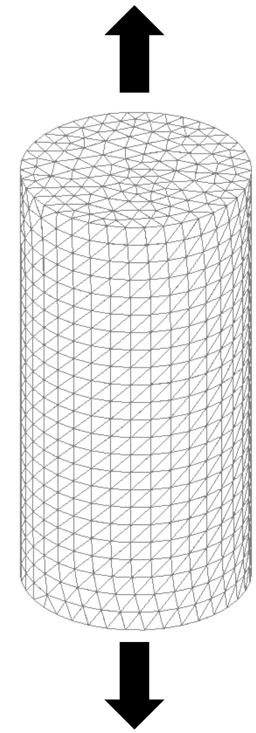
W: 35nm
H: 58nm



$Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (Vitreloy 1)

Property	Value
Shear Modulus	$\mu(T) = -0.004 * T + 37 [\mathrm{GPa}]$
Poisson's ratio	$\nu = 0.352$
Debye Temperature	$327 [\mathrm{K}]$
Activation Energy	$\Delta F(T) = 0.8 - 1.2 \times 10^{-29} * \mu(T) [J]$
STZ Volume	$\Omega_o = 1.6 - 2.0 [\mathrm{nm}^3]$

3D



D: 10nm
H: 20nm

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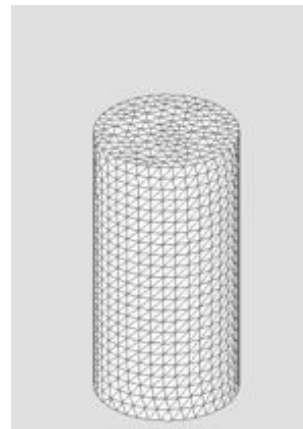
Characteristic Model Response

Vitreloy 1 ($Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$) Properties: G, ν, θ_D, ΔF

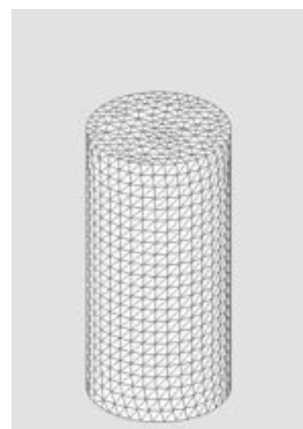
2D (Pure Shear)
35nm x 58nm

3D (Tension)
10nm x 20 nm

High T
Low σ



Low T
High σ



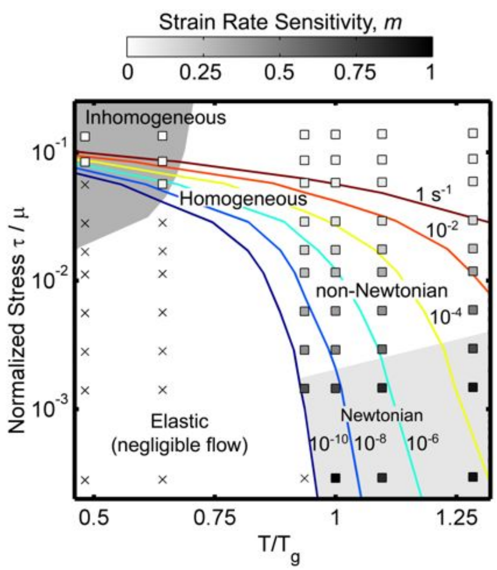
Homer, Schuh. Acta Mat. 2009.

Homer, Schuh. Model Simul Mater Sci Eng. 2010.

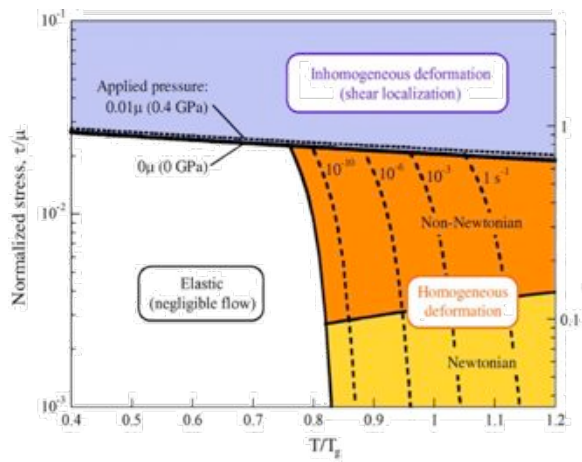
STZ Dynamics characteristic response

2D

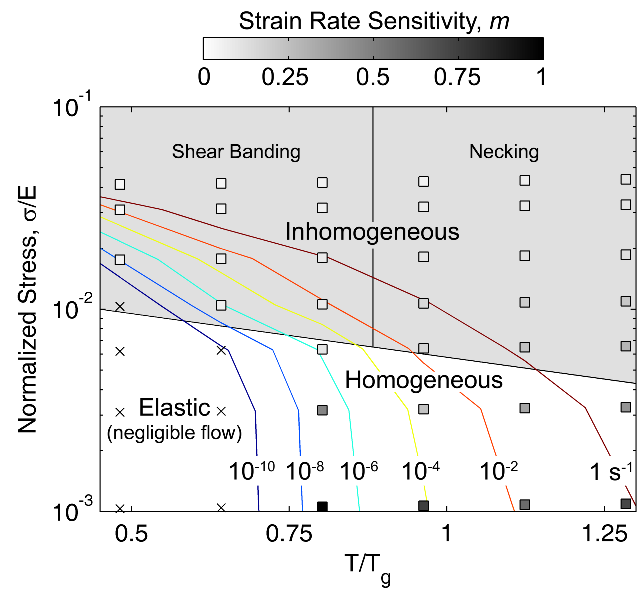
3D



Homer, Schuh. Acta Mat 2009.



Schuh et al. Acta Mat. 2007.



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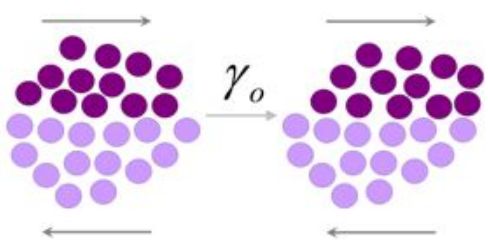

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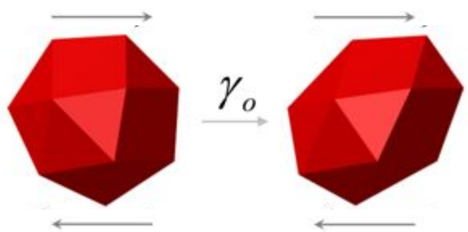
Presentation Topics

Amorphous Metals

Development & Validation



Kinetic Monte Carlo
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Moser, et al. Phil. Mag. 2006.

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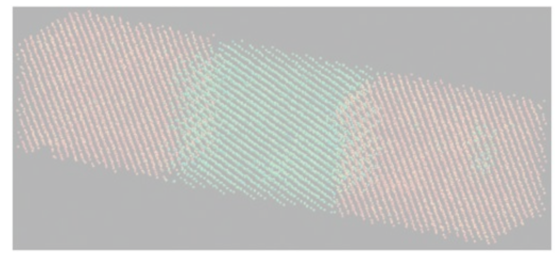
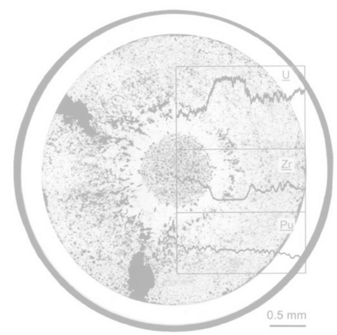


Janssens, et al. Nat. Mat. 2006.

Microstructure Evolution



Potts Monte Carlo

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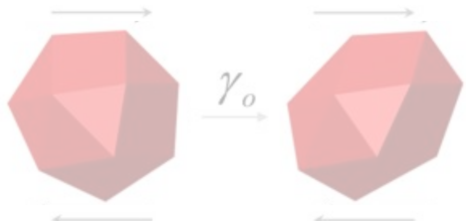

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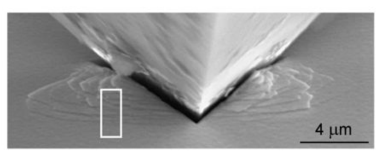

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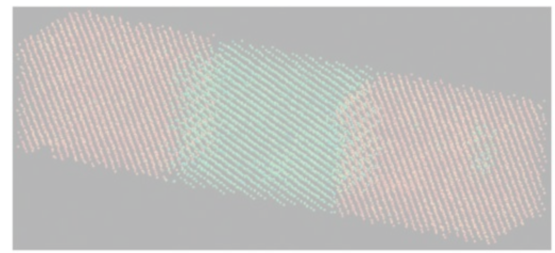

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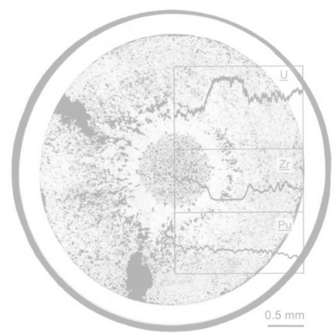


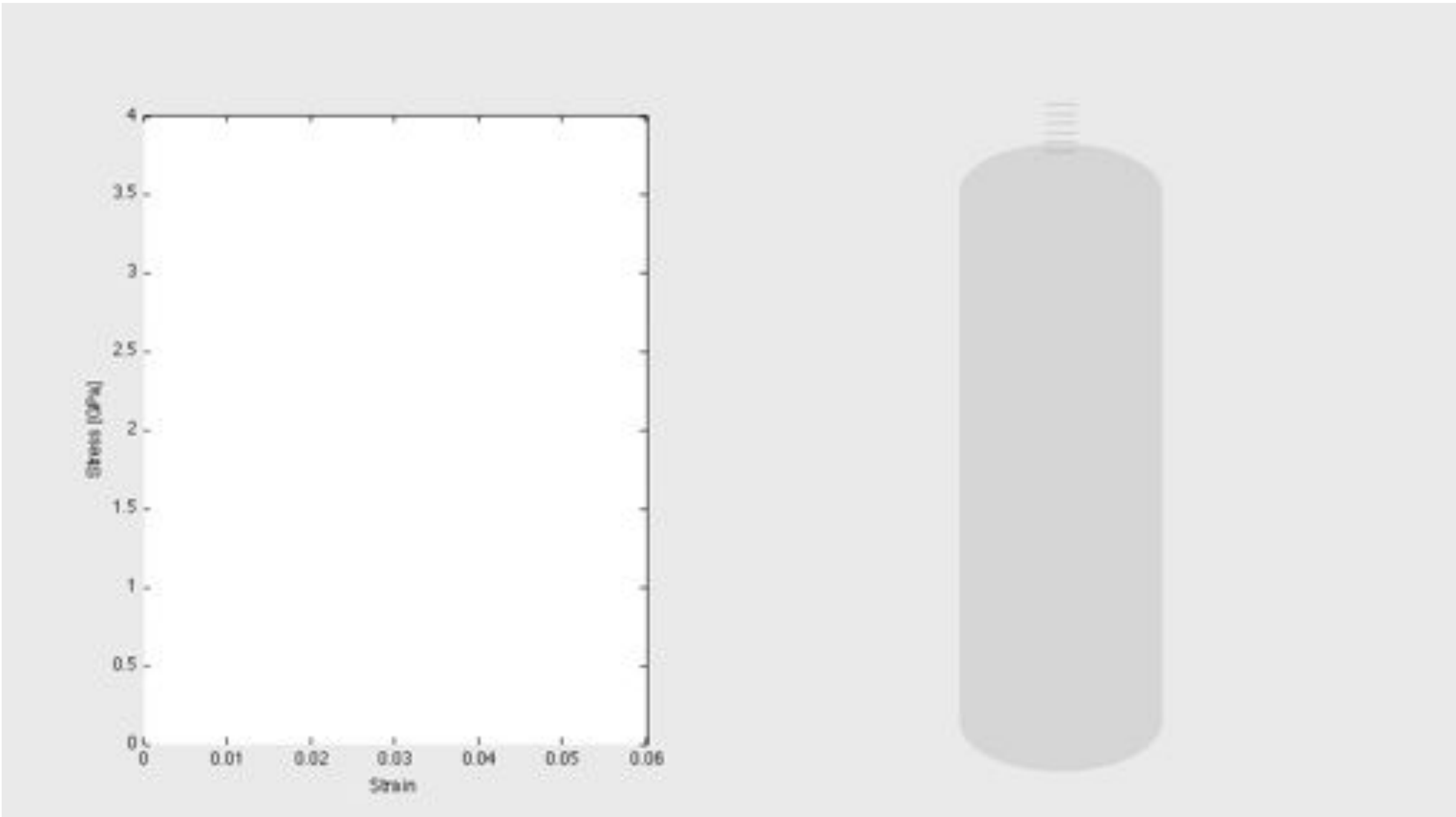
Potts Monte Carlo

Phase Field

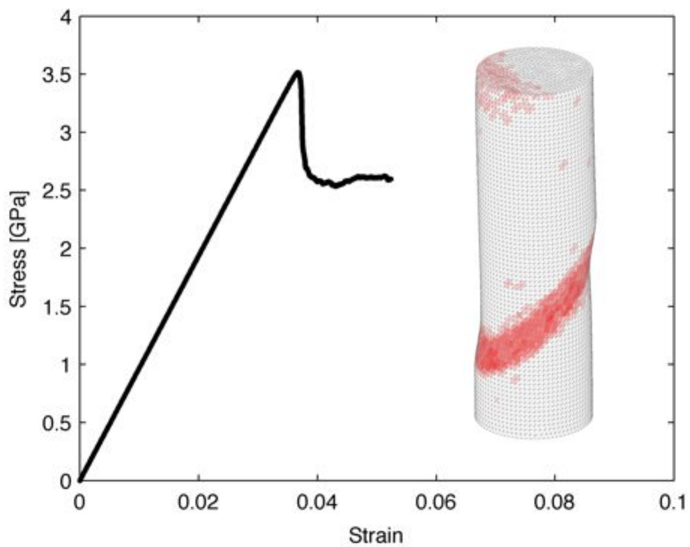
Kim, et al. J. Nucl. Mat. 2004.

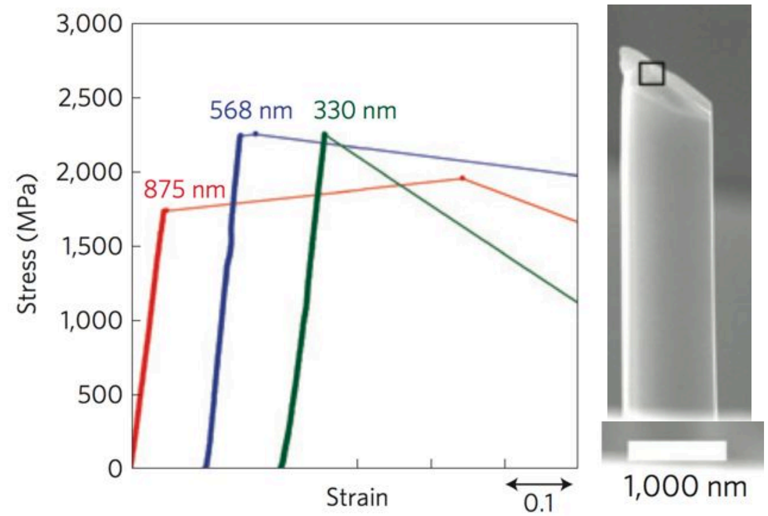
Constant Strain Rate Tensile Test

Strain Rate: 10^{-3} s^{-1} D: 20nm, H: 60nm



Model & Experimental Comparisons

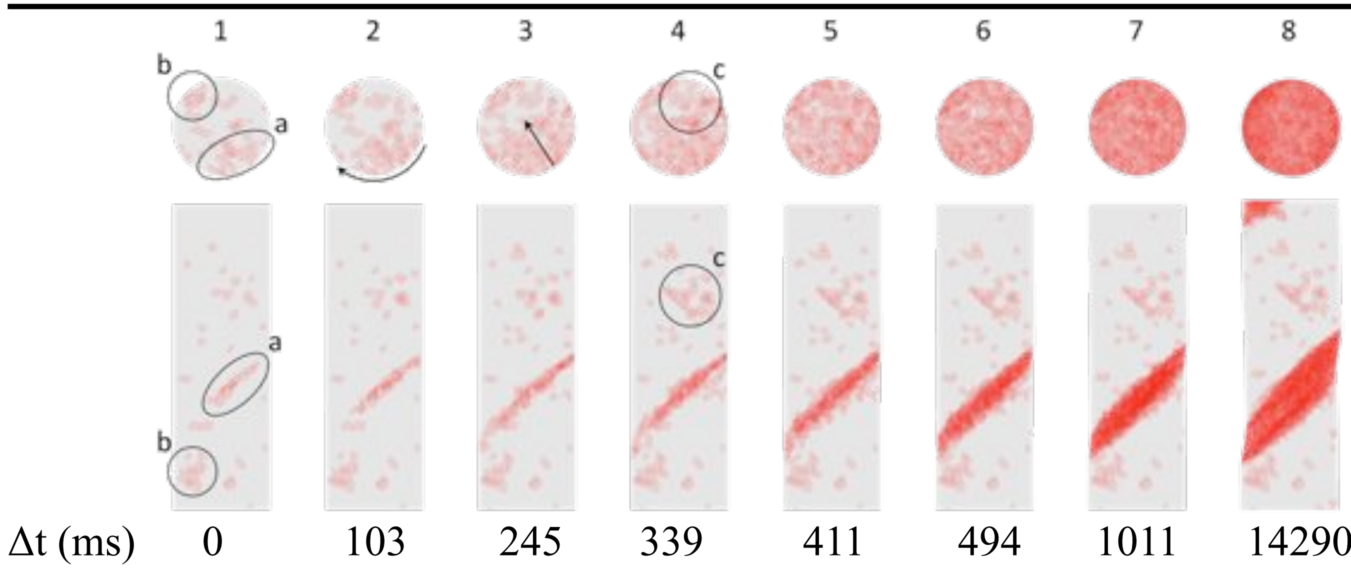


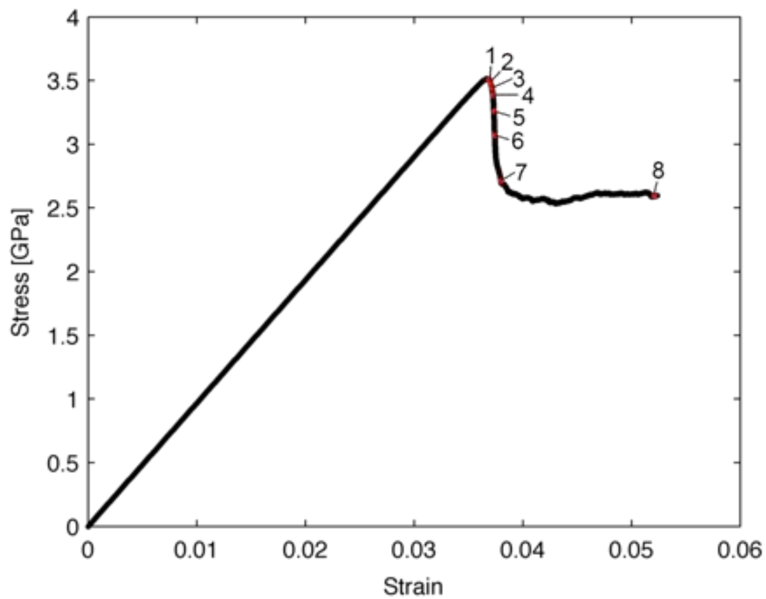


Jang, Greer. Nat. Mat. 2010.

Isolated Shear Localization Event

Details of shear localization event

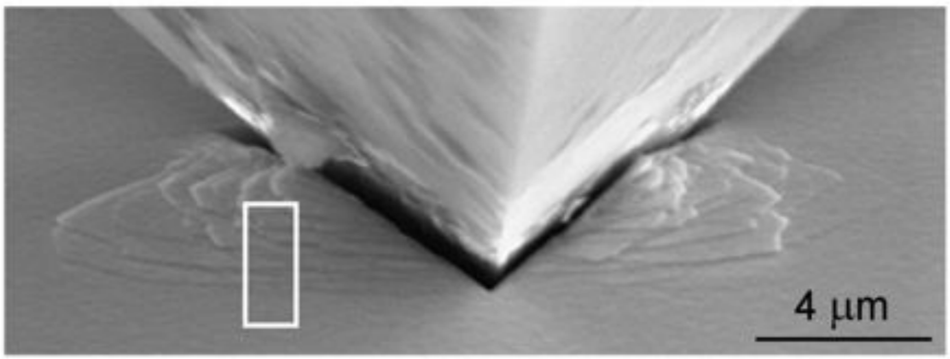




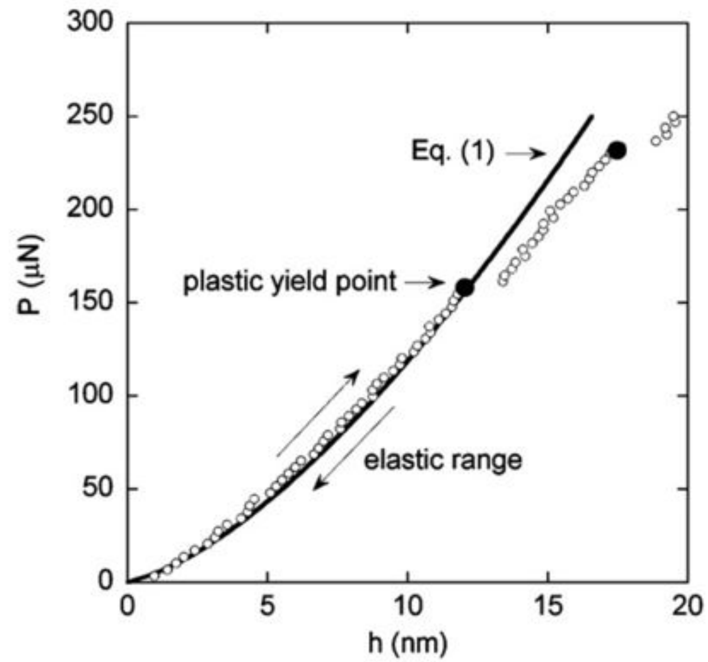
	Model	Experiment
Nucleation	Several possible sites	Areas of high free volume / stress concentrations
Path	Free Surface	Connected path of free volume / short range order
Velocity	Front: 0. 274 μm/s Band: 0.017 μm/s	40 μm/s [1] 317-336 μm/s [2] ≥ 5.3×10^5 μm/s [3]

[1] Neuhäuser. Scripta Mat. 1978.
[2] Chen, et al. APL 2009.
[3] Jiang, et al. JMR 2006.

Precision nanoindentation of a metallic glass

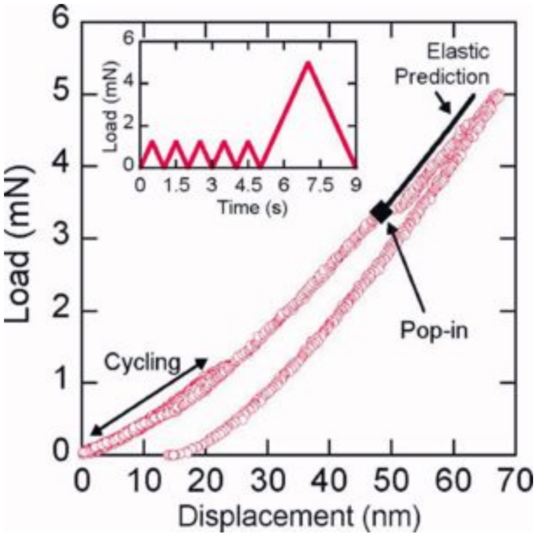


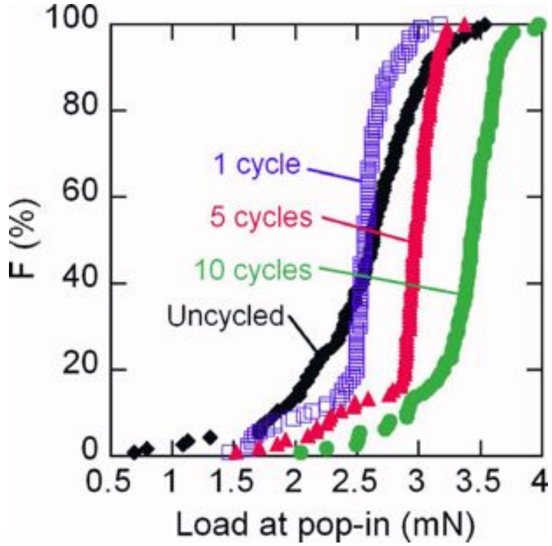
Moser, et al. Phil. Mag. 2006.



Packard, Schuh. Acta Mat. 2007.

Cyclic loading leads to nanoscale strengthening

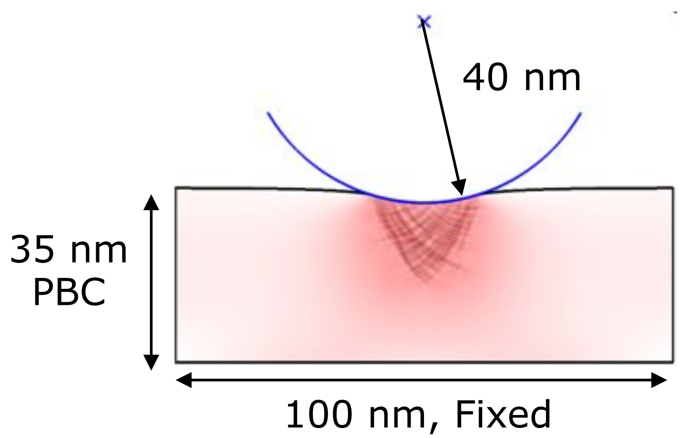




Packard et. al. APL. 2008.

- •Cycling load threshold
- •Act of cycling required
- •Saturation in strengthening

Packard, Homer, et al. Phil Mag. 2010.



Microplasticity (STZ activity)

- •Energetically plausible
- •Imperceptible activity
- •Low T kinetics – correct time
- •STZ activity leads to hardening

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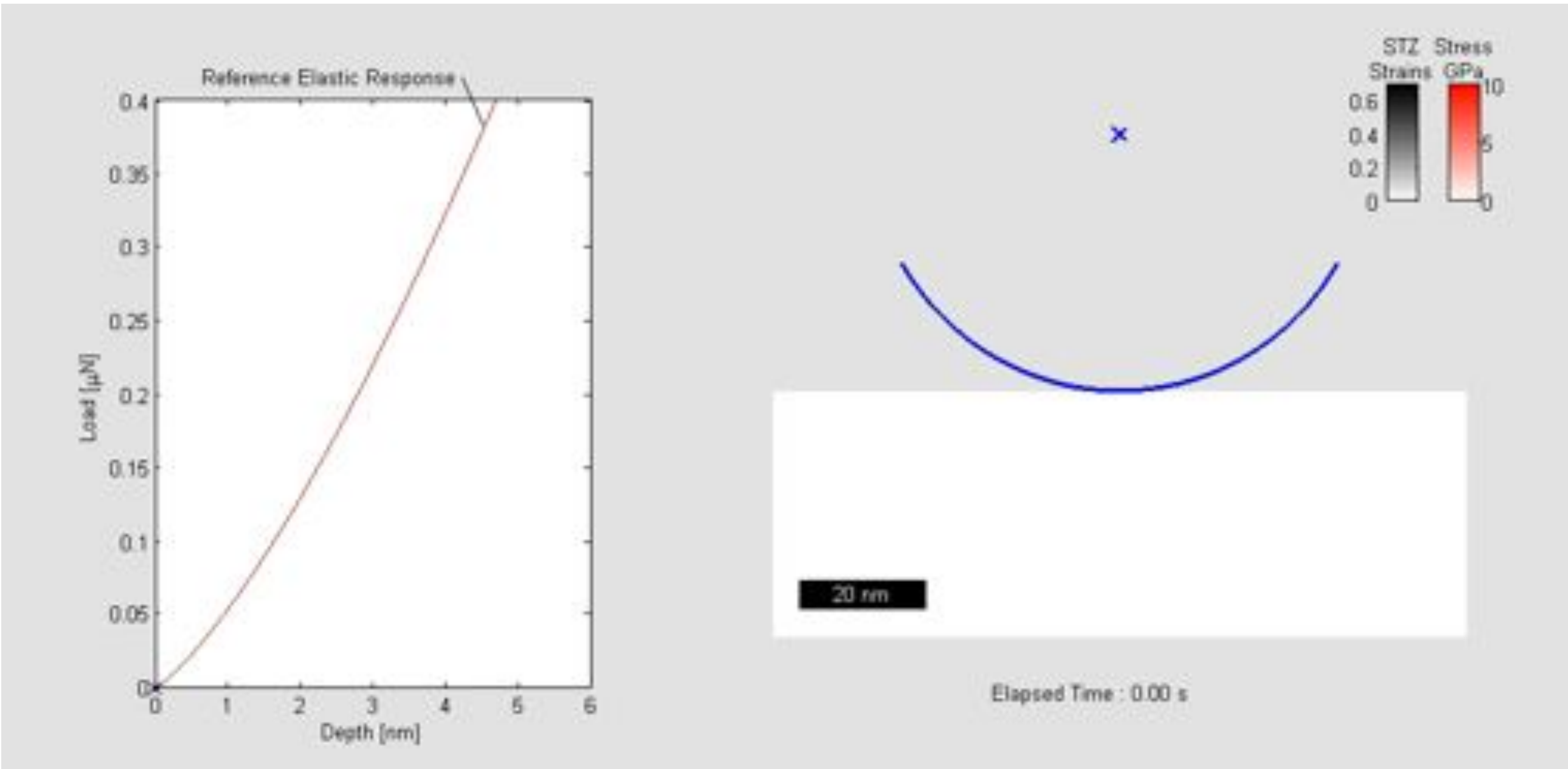
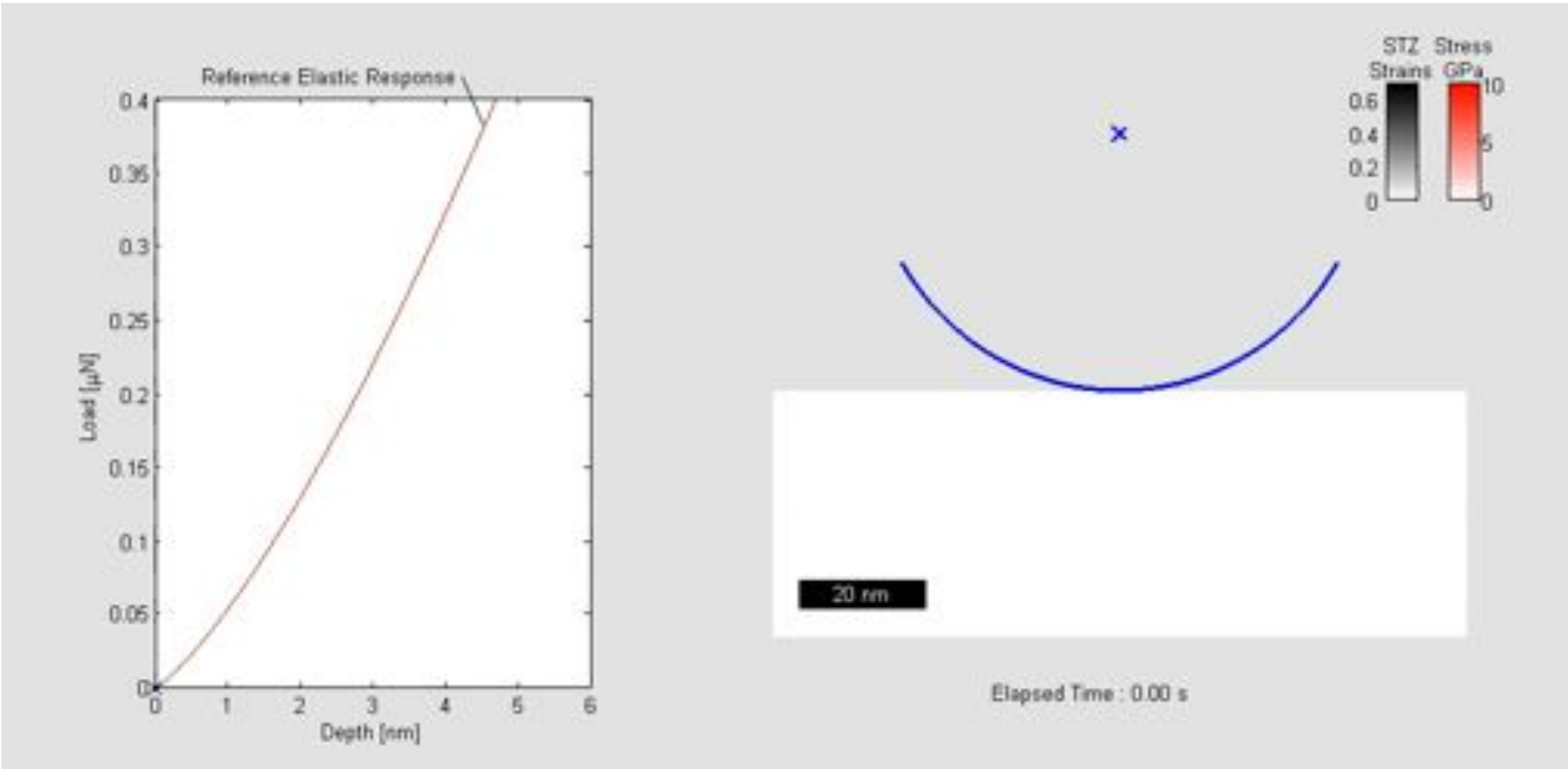
Monotonic loading of a metallic glass



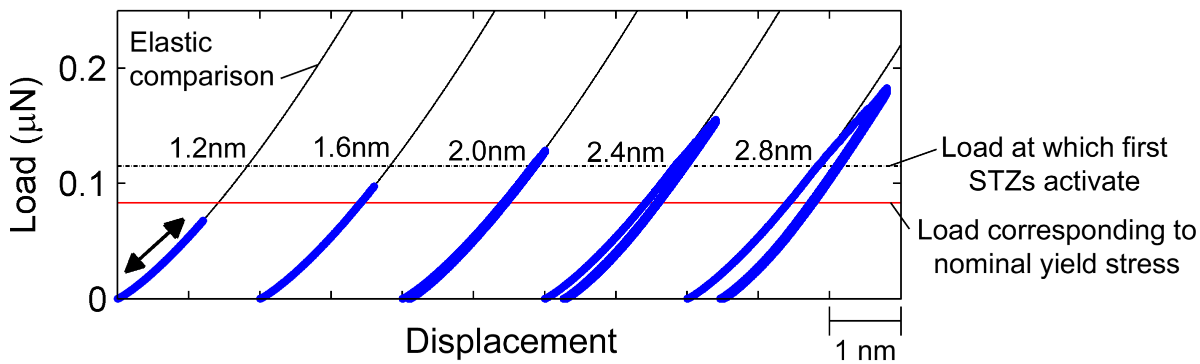
Packard, Homer, et al. Phil Mag. 2010.

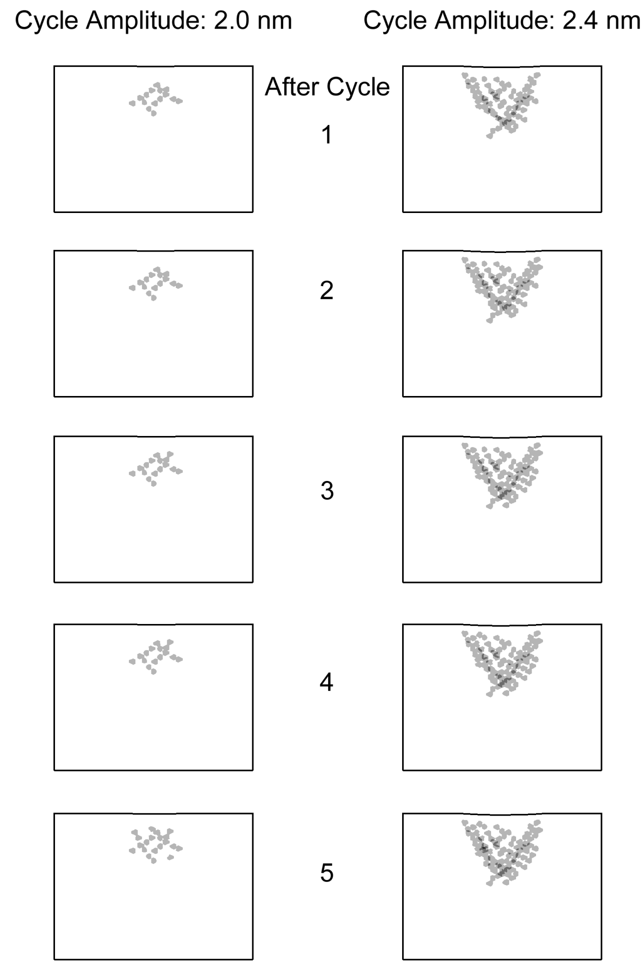
Effect of cycling indenter to a depth of 2.0 nm



Packard, Homer, et al. Phil Mag. 2010.

STZ activity is significant and undetectable



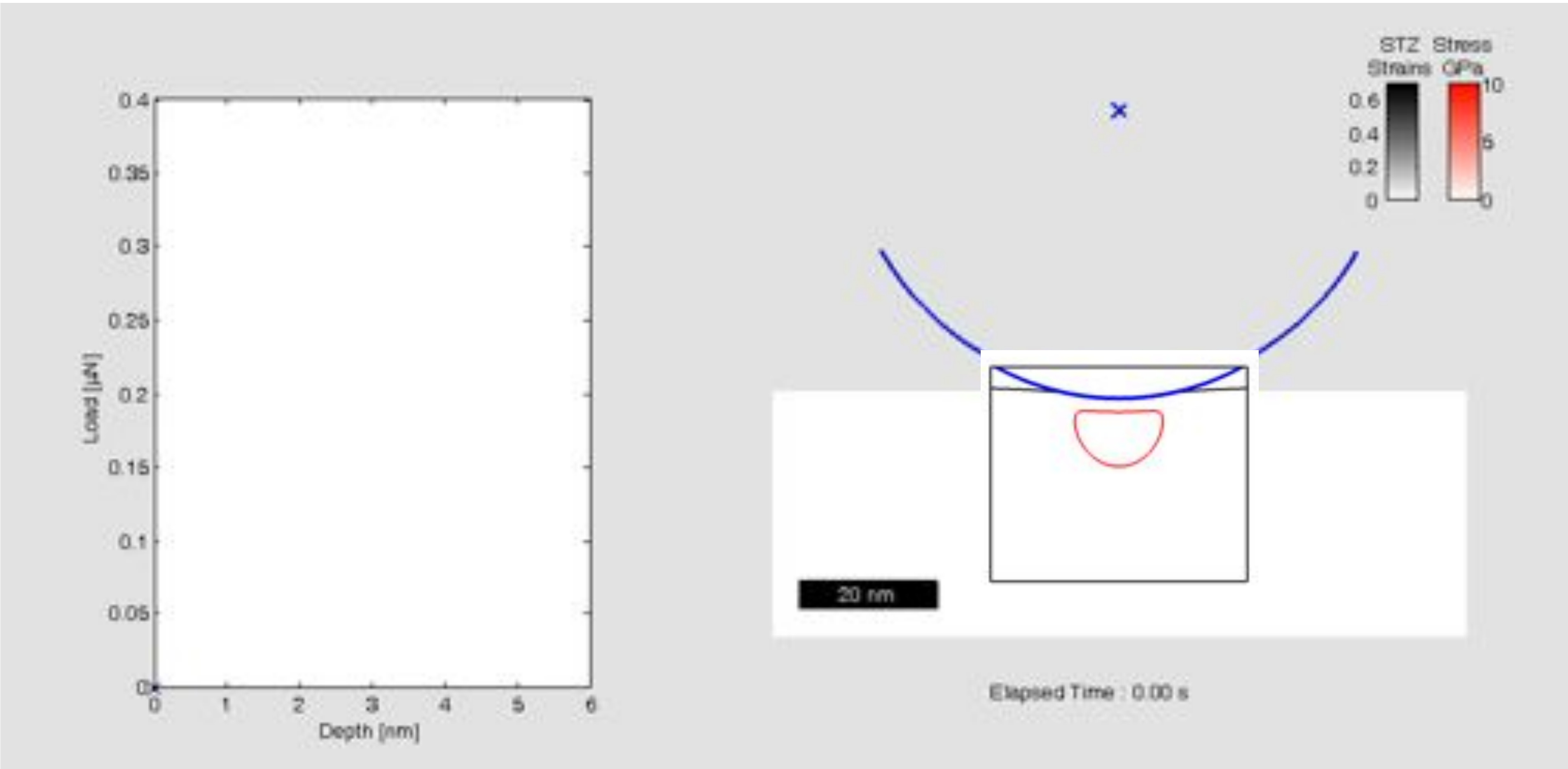


Microplasticity (STZ activity)

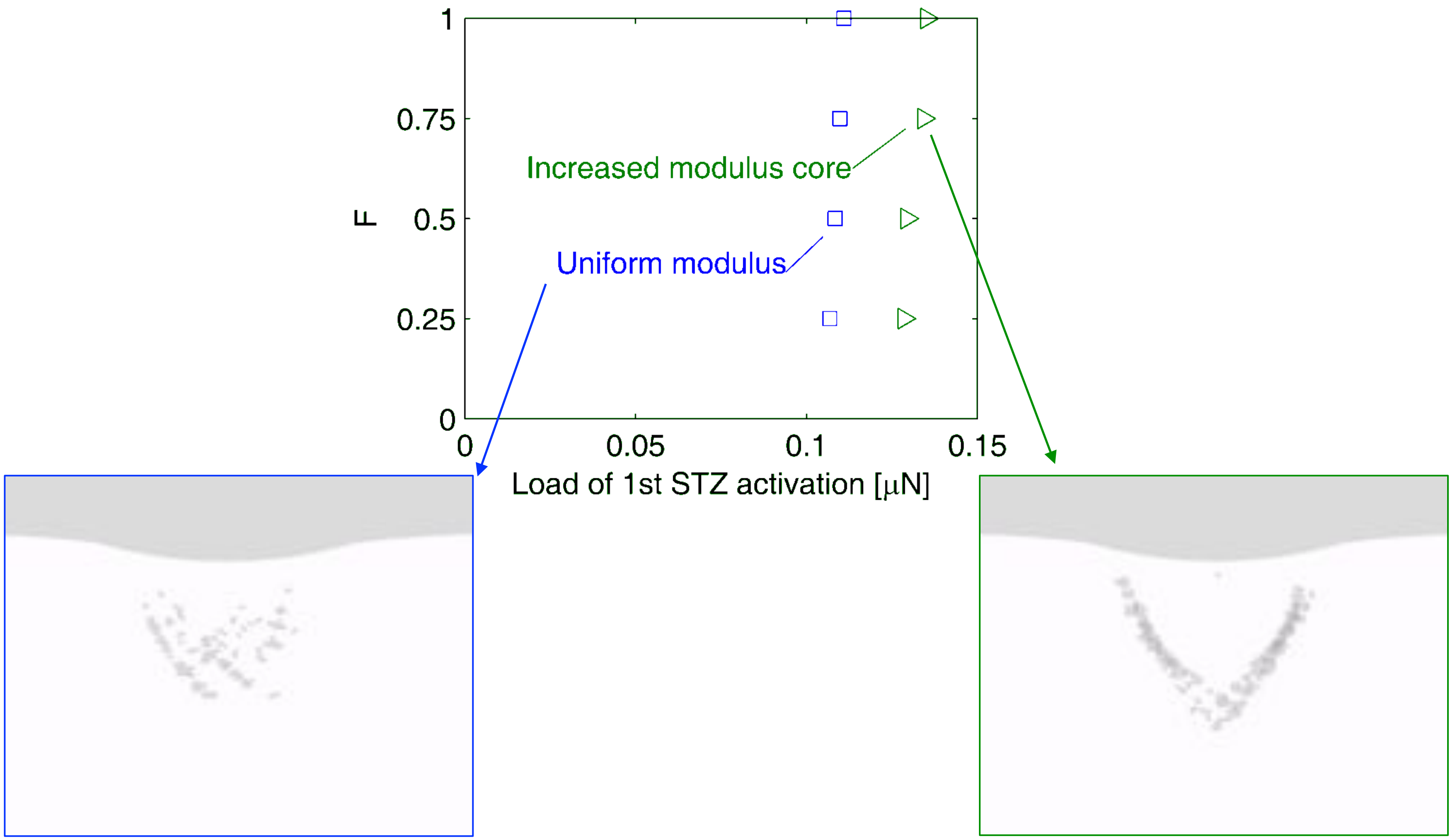
- •Energetically plausible
- •Imperceptible activity
- •Low T kinetics – correct time
- •STZ activity could lead to hardening

Packard, Homer, et al. Phil Mag. 2010.

Indentation of a strengthened metallic glass

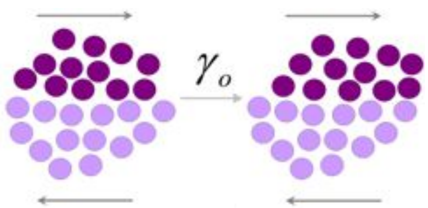


Strengthening a glass increases STZ load



STZ Dynamics Extensions

STZ Dynamics Model

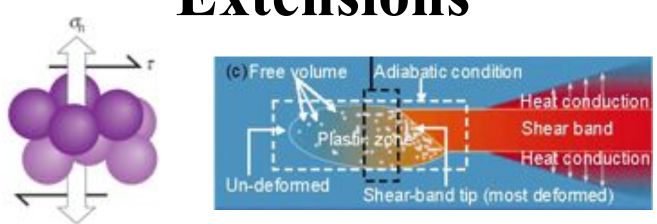


Redistribute stress

Isothermal

$$\dot{s} = \dot{s}(\tau, T)$$

Extensions



$$\dot{s} = \dot{s}(\tau, T, V_f, \sigma_n)$$

Schuh et al. Nat. Mat. 2003. Yang et al. APL. 2005.

Source Code

ABAQUS

MATLAB

MySQL

python

Fortran

C/C++

Parallel Processing

Open-Source

Parallel Processing

C/C++

LAMMPS

SPPARKS

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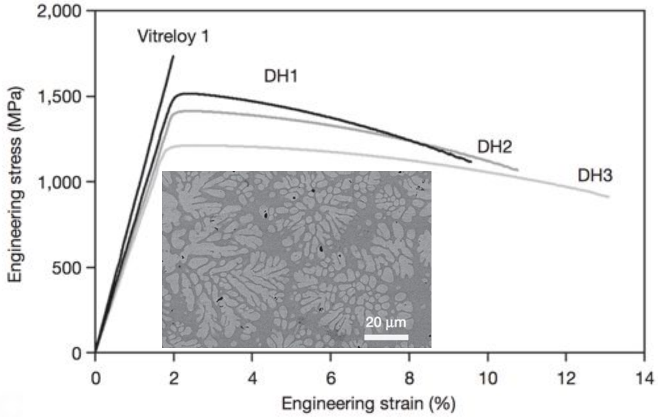
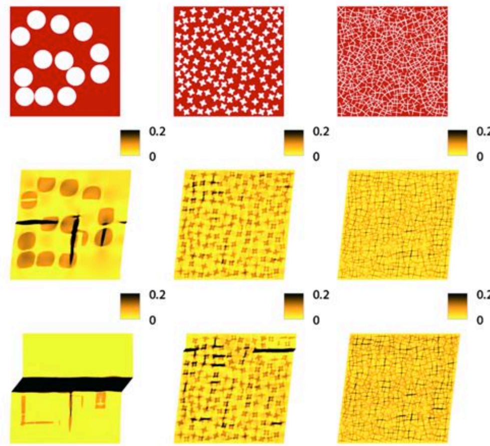
STZ Dynamics Extensions: Composites

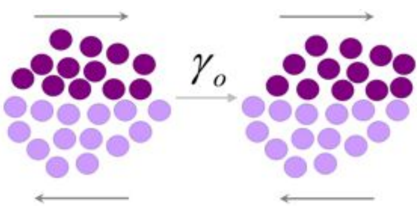
MGM Composites

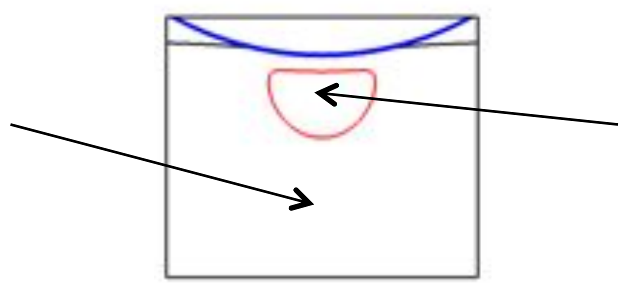


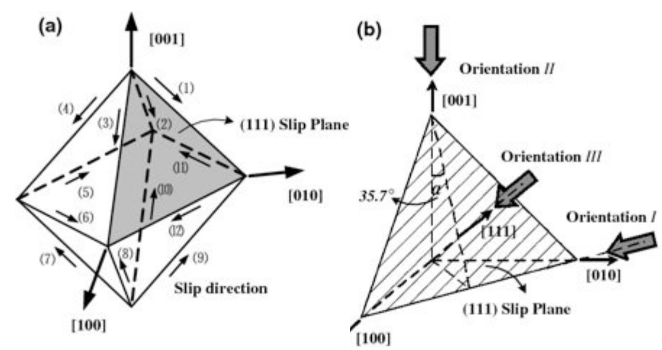
Hofmann et al. Nat. 2008.



Abdeljawad. et al. APL. 2011.





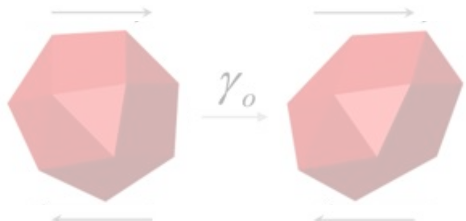


Li. et al. Nanoscale Res Lett. 2010.

Presentation Topics

Amorphous Metals

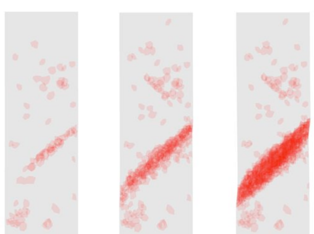
Development & Validation



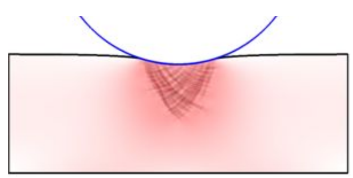
Kinetic Monte Carlo
Finite Element Analysis
2D & 3D

Applications

Shear Localization



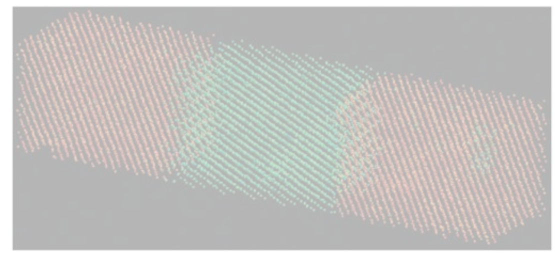
Nano-Indentation



Polycrystalline Metals

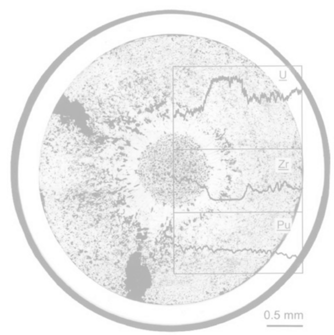
Grain Boundary Motion

Atomistic Simulations



Janssens, et al. Nat. Mat. 2006.

Microstructure Evolution



Potts Monte Carlo

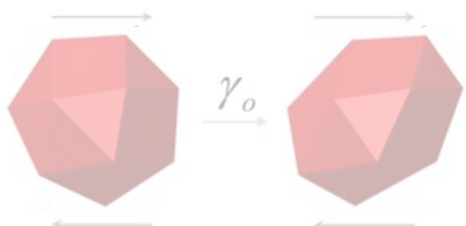
Phase Field

Kim, et al. J. Nucl. Mat. 2004.

Presentation Topics

Amorphous Metals

Development & Validation

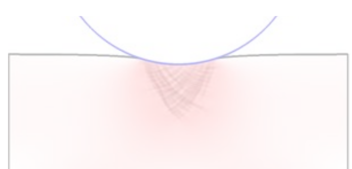


Kinetic Monte Carlo
Finite Element Analysis
2D & 3D

Applications

Shear Localization

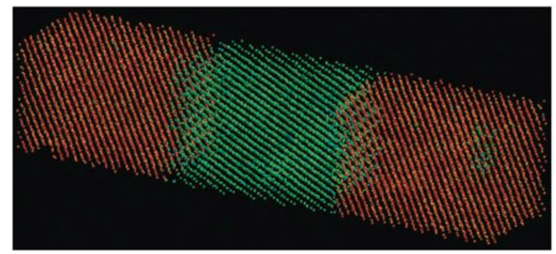
Nano-Indentation



Polycrystalline Metals

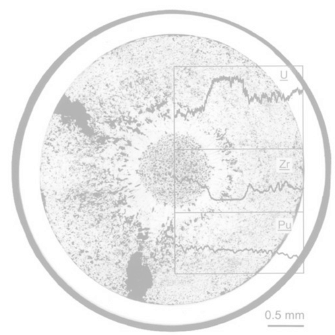
Grain Boundary Motion

Atomistic Simulations



Janssens, et al. Nat. Mat. 2006.

Microstructure Evolution



Potts Monte Carlo

Phase Field

Kim, et al. J. Nucl. Mat. 2004.

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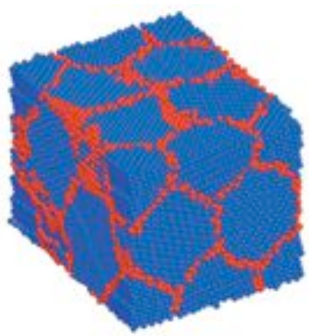
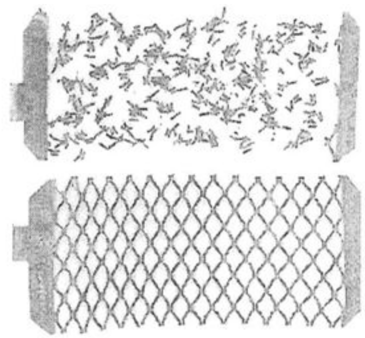
Grain Boundary Motion

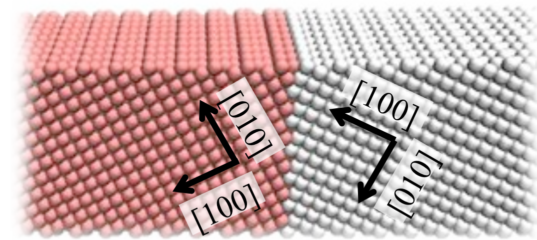


Schuh Group, MIT.



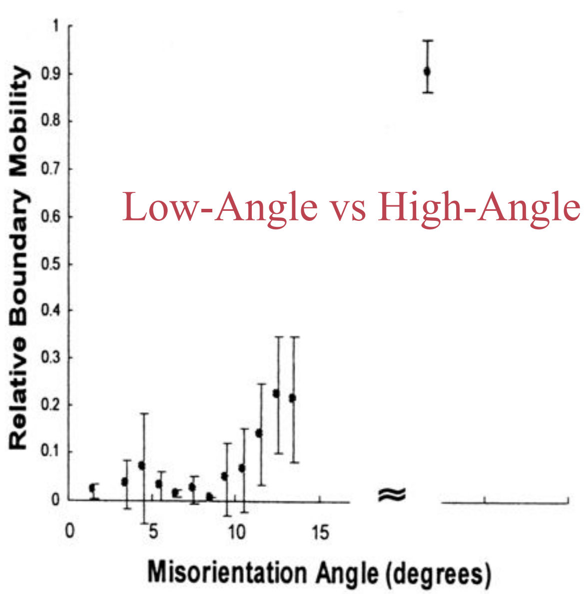
Palumbo, et al. JOM. 1998.

$$f\left(\Delta g, \hat{n}\right)$$



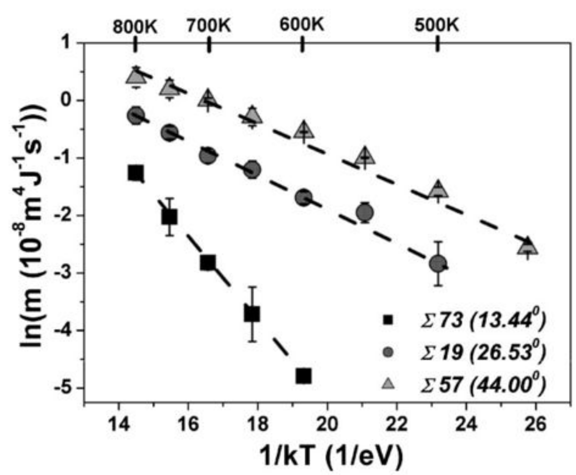
Misorientation space is 5-dimensional

Low-Angle vs High-Angle GBs



Yang, et al. Scripta Mat. 2001.

Thermally-Activated



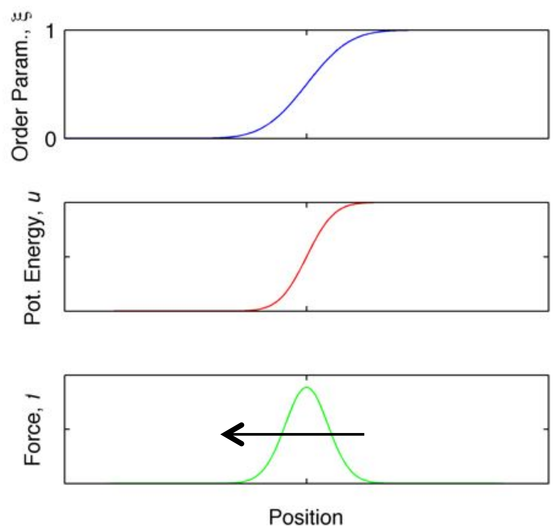
Zhou, et al. Steel Res. Int. 2011.

Synthetic Driving Force Molecular Dynamics

Pair Potential: $E_i = F_\alpha \sum_{i \neq j} \rho_\beta(r_{ij}) + \frac{1}{2} \sum_{i \neq j} \phi_{\alpha\beta}(r_{ij})$

Integrate Motion: (r_i, v_i, a_i, f_i)

Synthetic Driving Force

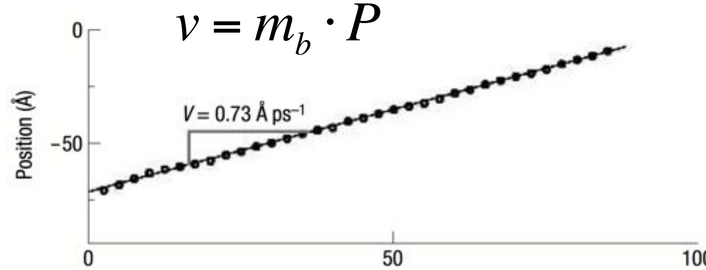


$\xi_i = \sum_j \left| r_j - r_j^I \right|$

$u_\xi = \frac{V}{2}\left(1 - \cos(2\xi_i)\right)$

$F(r_i) = -\frac{\partial u_\xi}{\partial r_i}$

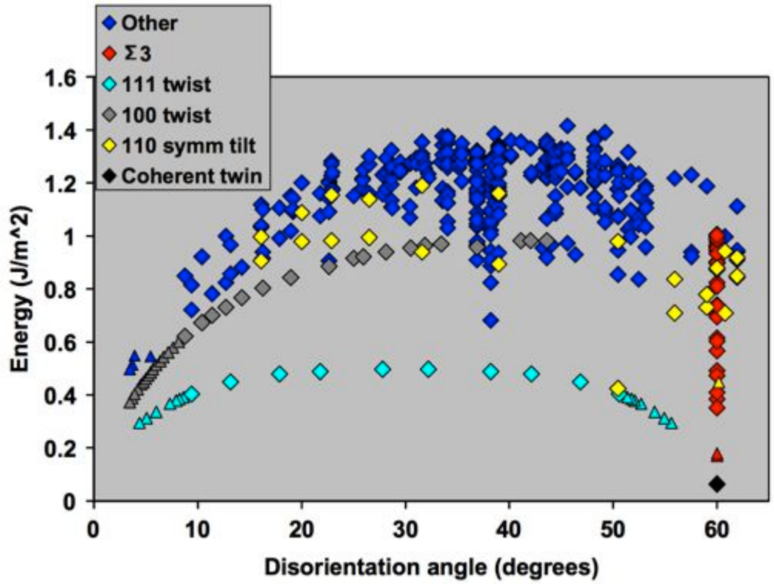
$v = m_b \cdot P$



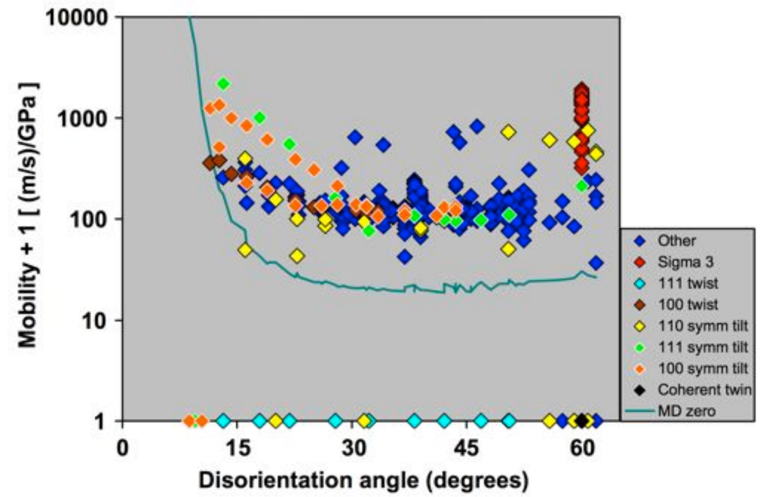
Janssens, et al. Nat. Mat. 2006.

Energy and Mobility of Grain Boundaries

388 Different Boundaries $f(\Delta g, \hat{n})$



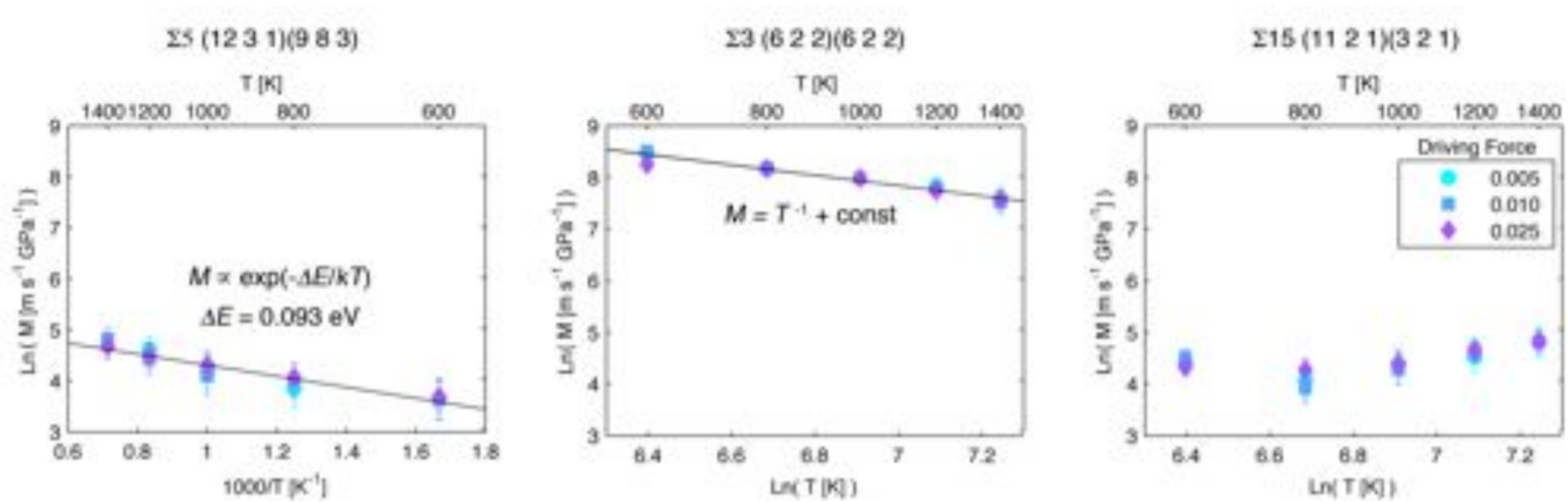
Olmsted, Foiles, et al. Acta Mat. 2009.

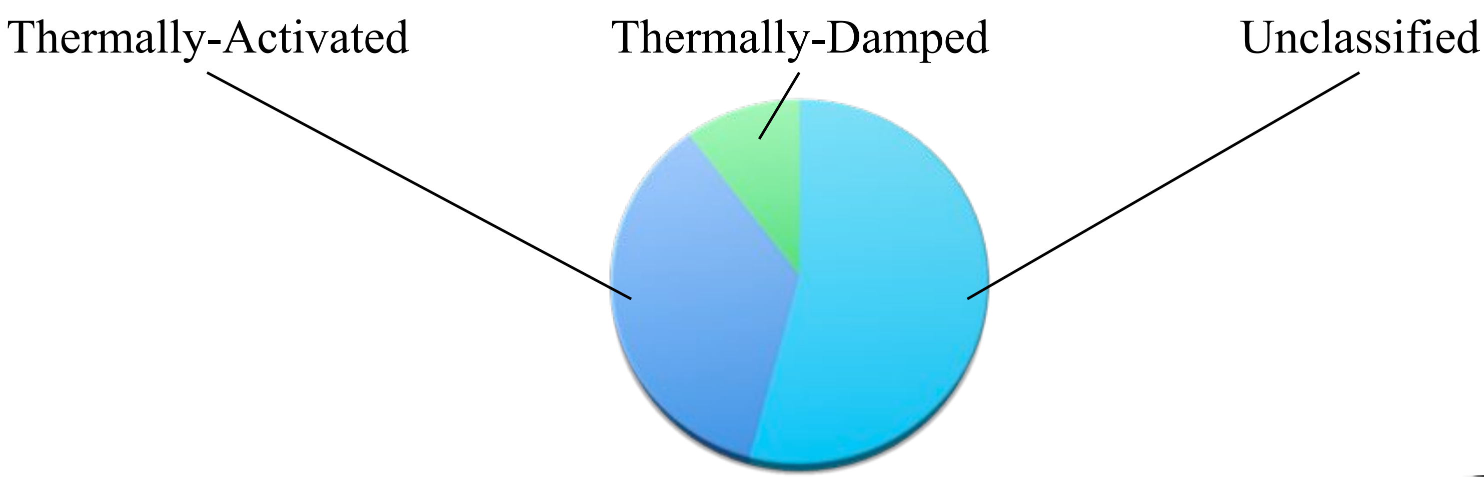


Olmsted, Holm, et al. Acta Mat. 2009.

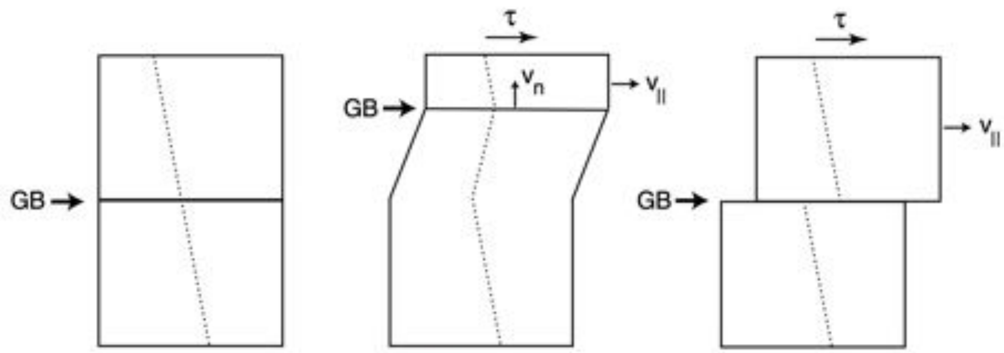
Mobility Temperature-Dependence: ~ 10,000 Simulations

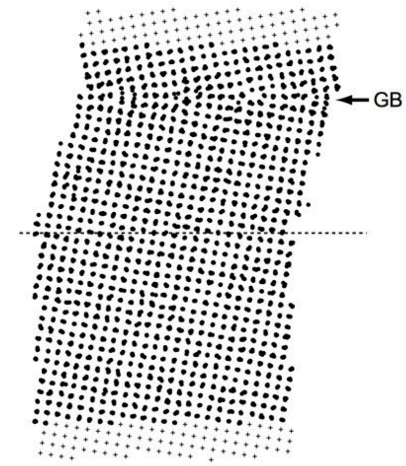
Temperature-Dependent Boundary Motion

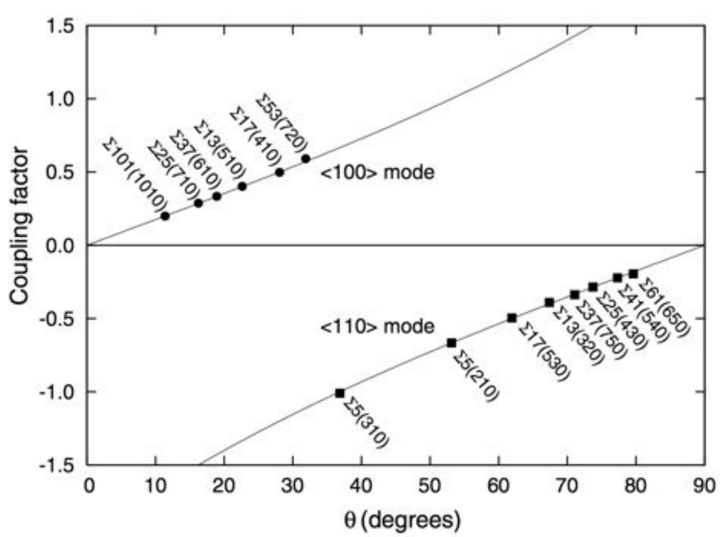


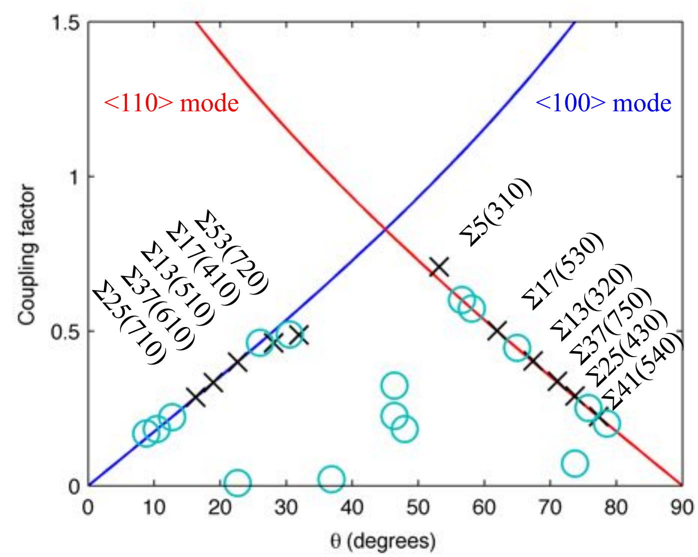


Shear-Coupled Boundary Motion



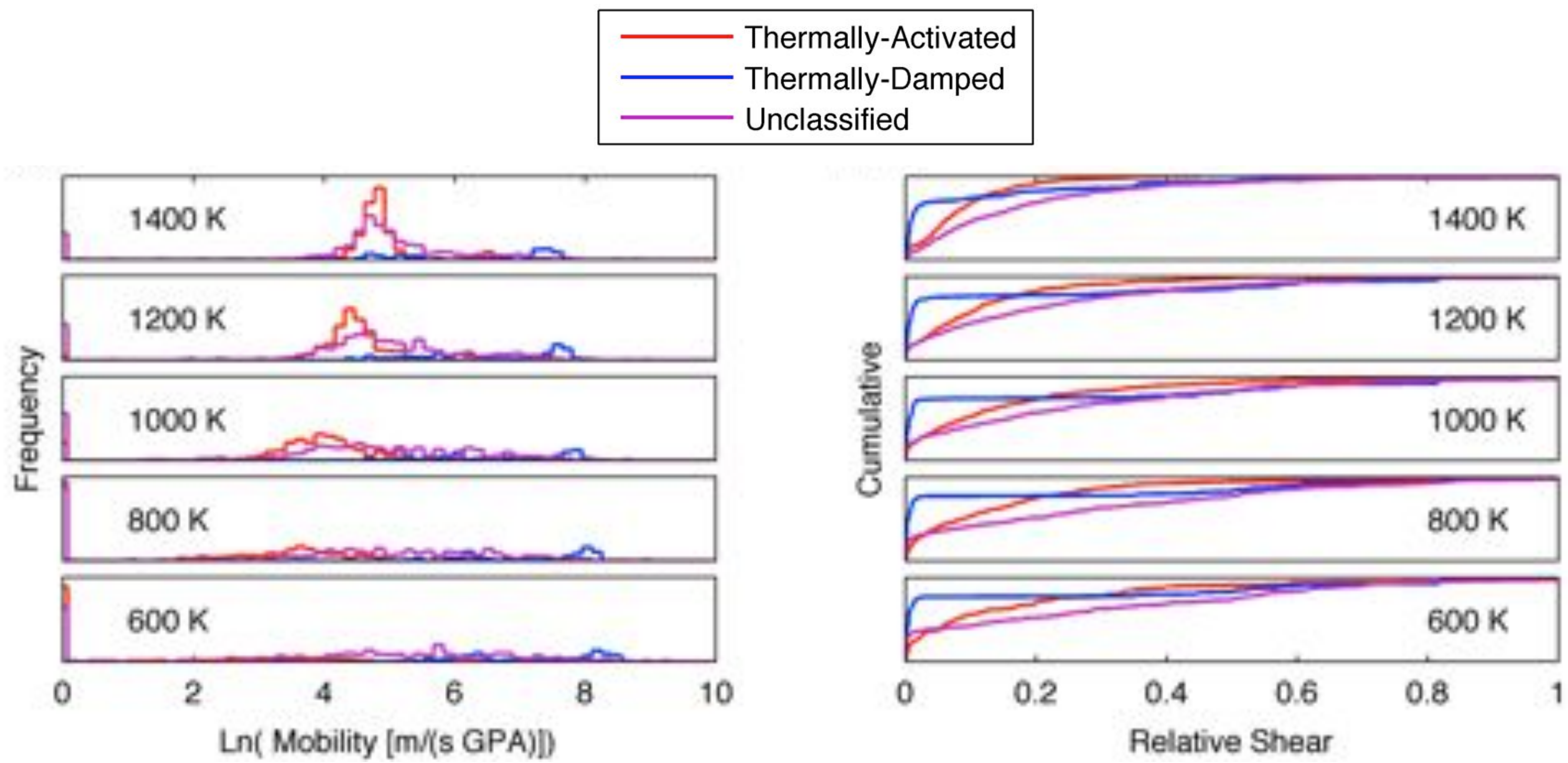






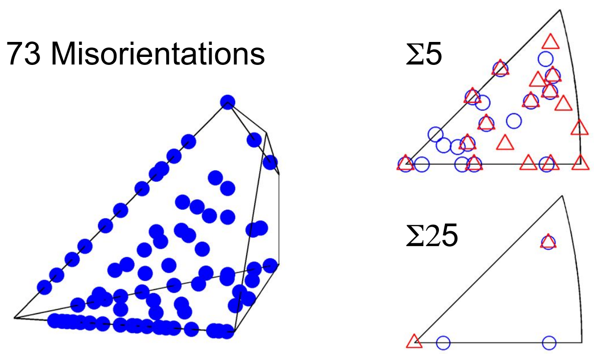
Cahn, et al. Acta Mat. 2006.

Mobility and Shear Distributions

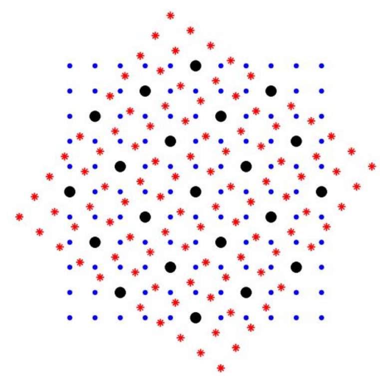


Future Grain Boundary Research

Boundary Sampling



CSL Determination



$$f\left(\Delta g\right)$$

$$\Delta\theta \le 15^{\circ}\,\Sigma^{-5/6}$$

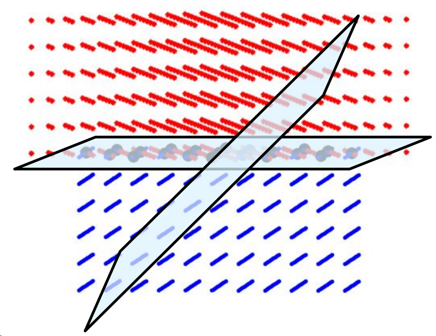
Sampling & Fitting

Uniform Sampling

$$E\left(\Delta g,\hat{n}\right) = \sum_{i,j,k}\sum_{l,m} a_{ijk}^{lm} T_i^{jk}\left(\Delta g\right) k_l^m\left(\hat{n}\right)$$

$$E\left(\Delta g\right) = \iint_{S^2} \sum_{i,j,k}\sum_{l,m} a_{ijk}^{lm} k_l^m\left(\hat{n}\right)$$

Consider Inclination

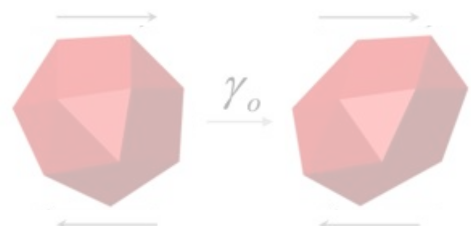


$$f\left(\Delta g,\hat{n}\right)$$

Presentation Topics

Amorphous Metals

Development & Validation

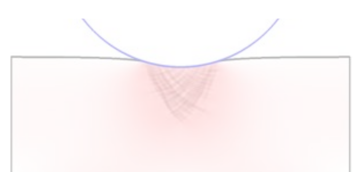


Kinetic Monte Carlo
Finite Element Analysis
2D & 3D

Applications

Shear Localization

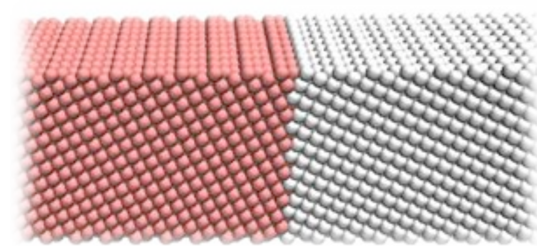
Nano-Indentation



Polycrystalline Metals

Grain Boundary Motion

Atomistic Simulations



Microstructure Evolution

Potts Monte Carlo

Phase Field

Kim, et al. J. Nucl. Mat. 2004.

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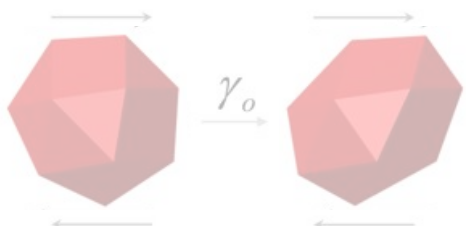
Presentation Topics

Amorphous Metals

Development & Validation



Kinetic Monte Carlo
Finite Element Analysis
2D & 3D

Applications

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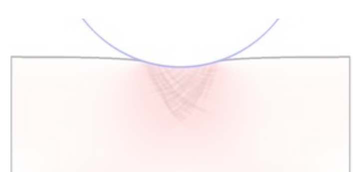

Polycrystalline Metals

Grain Boundary Motion

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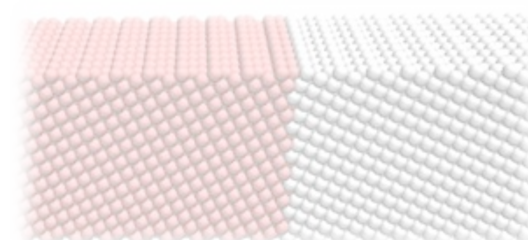
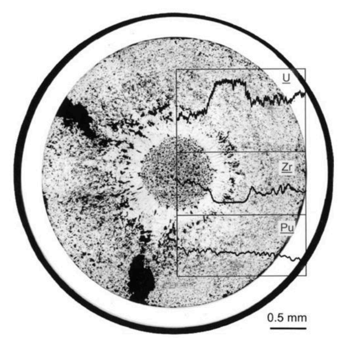


Microstructure Evolution



Kim, et al. J. Nucl. Mat. 2004.

Potts Monte Carlo

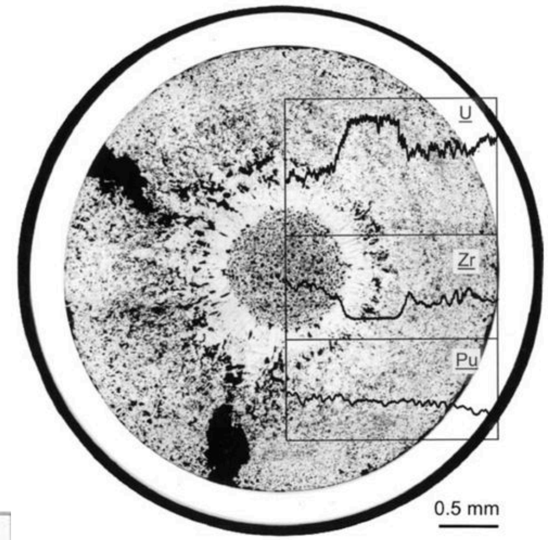
Phase Field

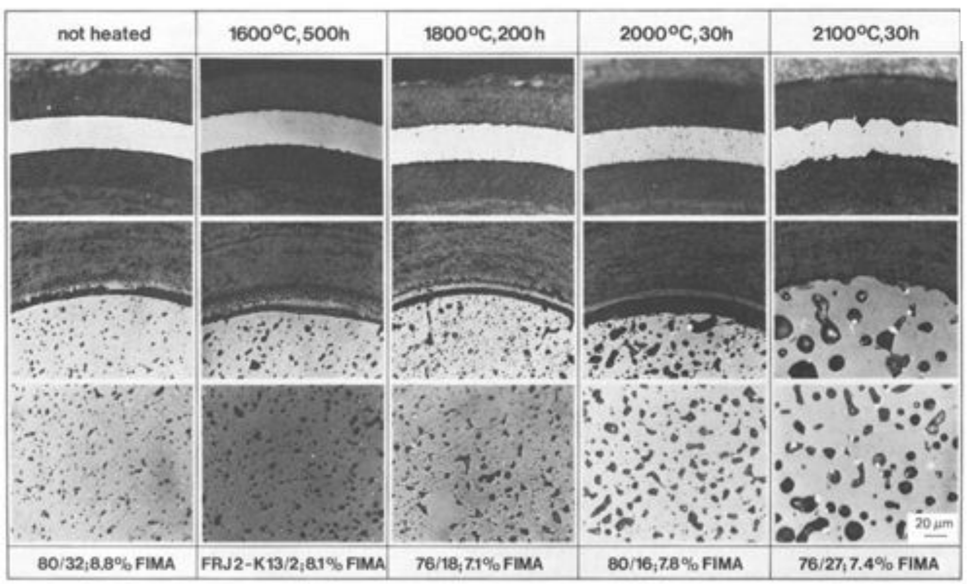
Sandia National Laboratories

Extreme Environments of Nuclear Power

Irradiation & Thermal Effects

- Fission Gas Generation
- Damage / Plasticity
- Impurity Fission Bi-Products
- Diffusion
- Creep
- Chemical attack between cladding and fuel





Combined approach of modeling techniques

Phase-Field

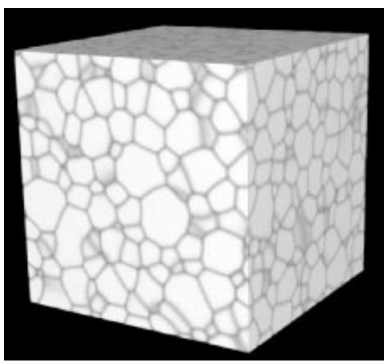
- Deterministic Continuum Model
- Smoothly varying fields
- Diffuse Interfaces
- Computationally expensive

Potts Monte Carlo

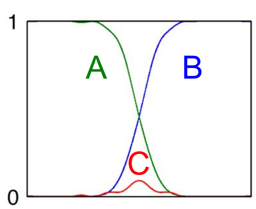
- Statistical-Mechanical Model
- Discrete Particles
- Sharp Interfaces
- Less expensive

Combined Model

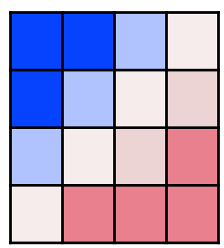
- Potts: Grain evolution
- PF: Concentration evolution
- Balance resolution / efficiency

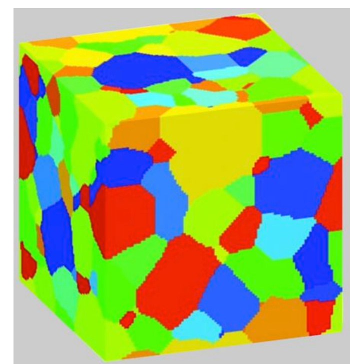


Chen. Annu Rev. Mat. Res. 2002.



A	A	A	B
A	A	B	B
A	C	B	B
C	C	C	C





Holm. et al. JOM. 2001.

A	A	A	B
A	A	B	B
A	C	B	B
C	C	C	C

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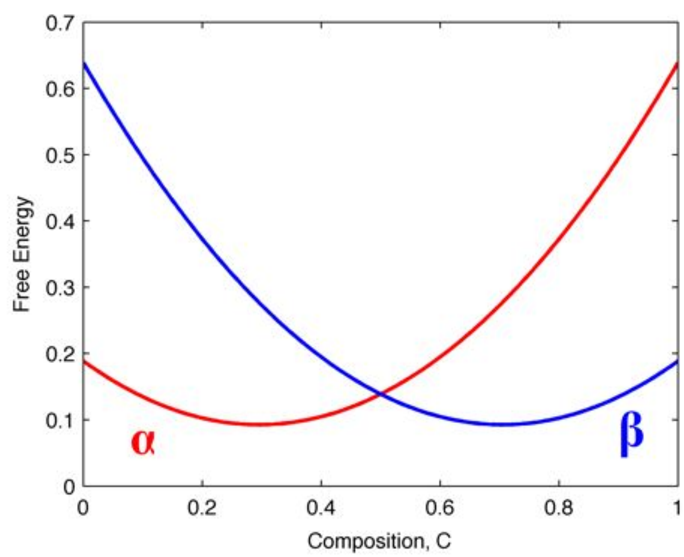
Details of the Combined Model

Combined Model Energetics

$$E_{hyb} = \sum_{i=1}^{N}\left(E_v(q_i,C) + \frac{1}{2}\sum_{j=1}^{n} J(q_i,q_j)\right) + \int \kappa_c (\nabla C)^2 dV$$

$$E_v = \gamma\left[(C-C_1)^2 + (C_2-C)^2\right] + a_1(C-C_3)^2 q_\alpha + a_2(C_4-C)^2 q_\beta$$



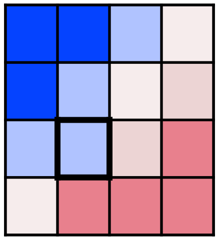
Potts Evolution

$$P = \begin{cases} \exp\left(-\frac{\Delta E}{k_B T}\right) & \text{for } \Delta E > 0 \\ 1 & \text{for } \Delta E \le 0 \end{cases}$$

A	A	A	B
A	A	B	B
A	A	B	B
C	C	C	C

Phase-Field Evolution

$$\frac{\partial C}{\partial t} = M_c\left(\nabla^2 \frac{\partial E_v}{\partial C} - \kappa_c \nabla^4 C\right)$$



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Coupled Potts – Phase Field Simulations

Combined Model Energetics

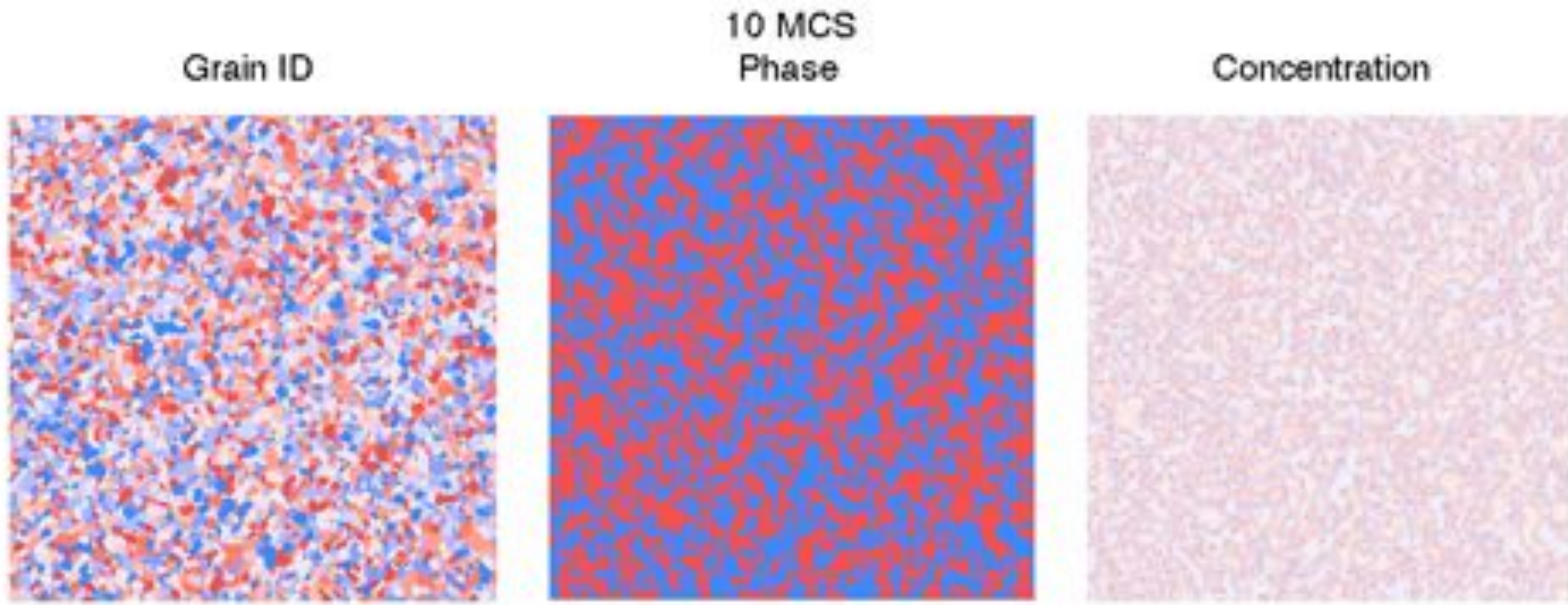
$$E_{hyb} = \sum_{i=1}^{N}\left(E_v(q_i, C) + \frac{1}{2}\sum_{j=1}^{n} J(q_i, q_j)\right) + \int \kappa_c (\nabla C)^2 dV$$

Potts Evolution

$$P = \begin{cases} \exp\left(-\frac{\Delta E}{k_B T}\right) & \text{for } \Delta E > 0 \\ 1 & \text{for } \Delta E \leq 0 \end{cases}$$

Phase-Field Evolution

$$\frac{\partial C}{\partial t} = M_c\left(\nabla^2 \frac{\partial E_v}{\partial C} - \kappa_c \nabla^4 C\right)$$



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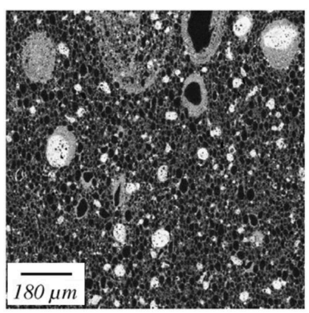
Future Nuclear Fuels Research

Potts – Phase Field

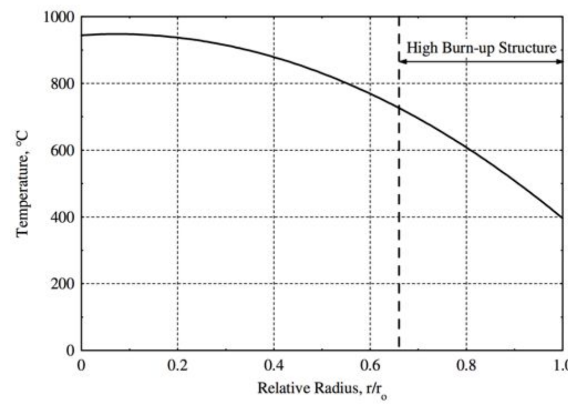
2-Phase Nuclear Fuel

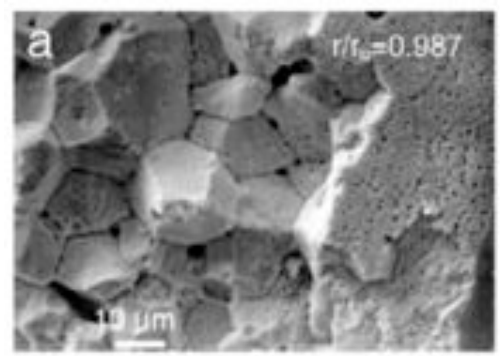


Oudinet. et. al. J. Nucl. Mat. 2008.

Thermal Effects

Walker. et al. J. Nucl. Mat. 2006.



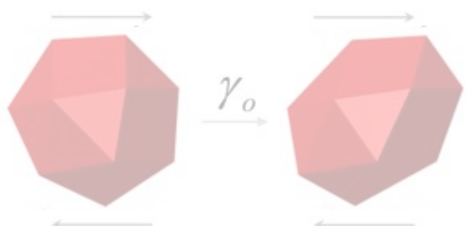


Spino. et al. J. Nucl. Mat. 2008.

Presentation Topics

Amorphous Metals

Development & Validation

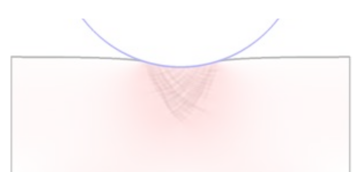


Kinetic Monte Carlo
Finite Element Analysis
2D & 3D

Applications

Shear Localization

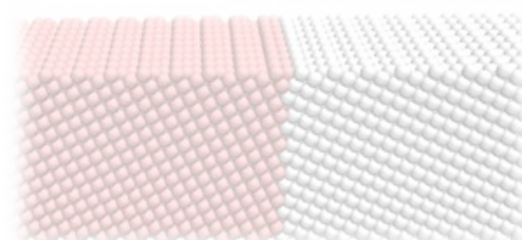
Nano-Indentation



Polycrystalline Metals

Grain Boundary Motion

Atomistic Simulations



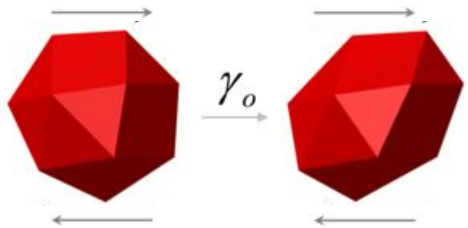
Microstructure Evolution

Sandia National Laboratories

Presentation Topics

Amorphous Metals

Development & Validation



Kinetic Monte Carlo
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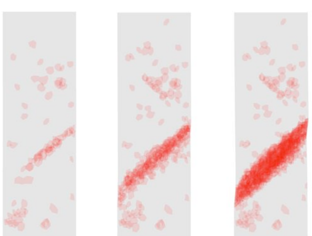
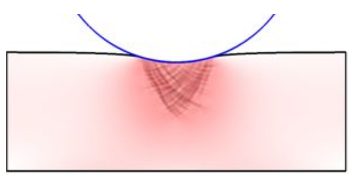


Nano-Indentation



Polycrystalline Metals

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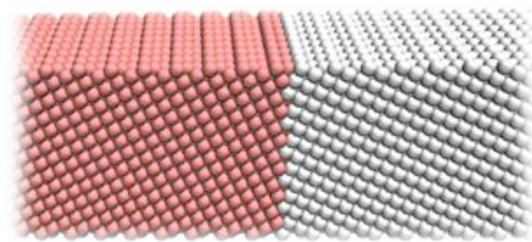

Microstructure Evolution

Sandia National Laboratories

Collaboration & Credit

Amorphous Metals

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Experiments
- Corrine E Packard
- Nassar Al-Aqeeli

Polycrystalline Metals

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MD Simulations
- David L Olmsted

Questions