# Rate-limited deformation mechanisms in nanocrystalline metals

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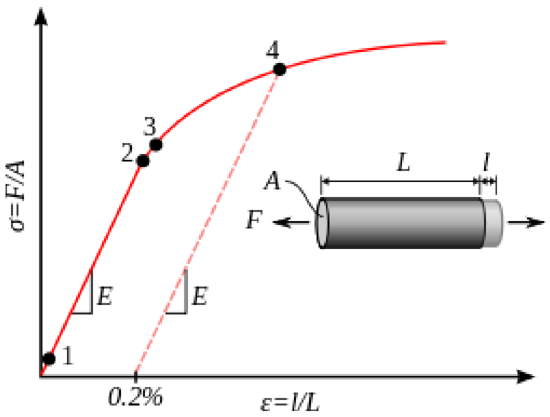
# Yield stress

## Yield (engineering)

From Wikipedia, the free encyclopedia

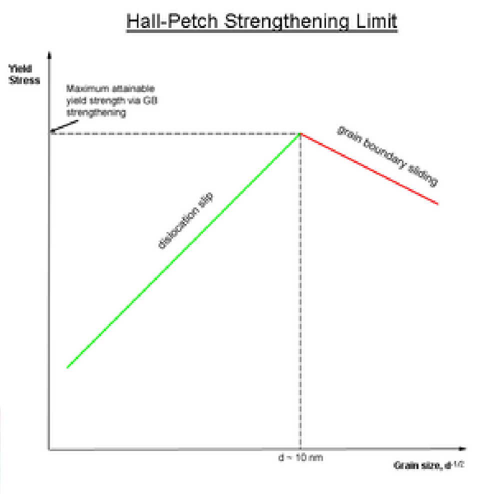
A **yield strength** or **yield point** of a material is defined in engineering and materials science as the stress at which a material begins to deform plastically. Prior to the yield point the material will deform elastically and will return to its original shape when the applied stress is removed. Once the yield point is passed, some fraction of the deformation will be permanent and non-reversible.



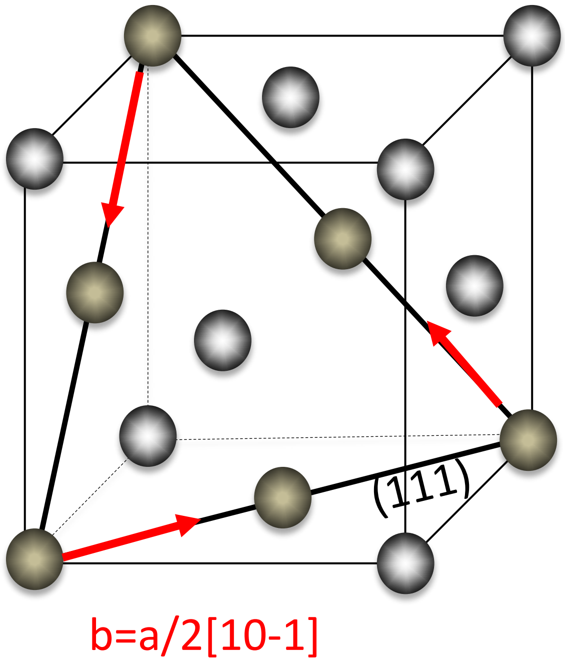

## Grain boundary strengthening

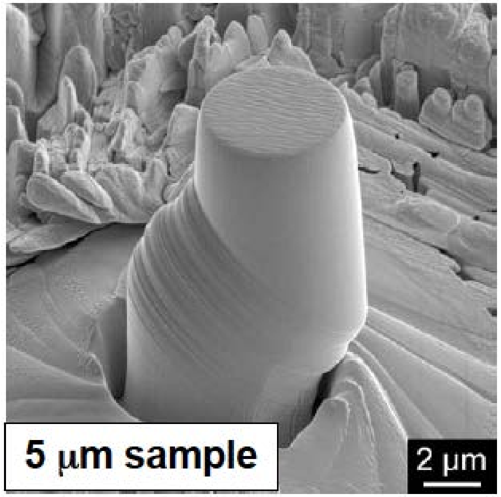
From Wikipedia, the free encyclopedia

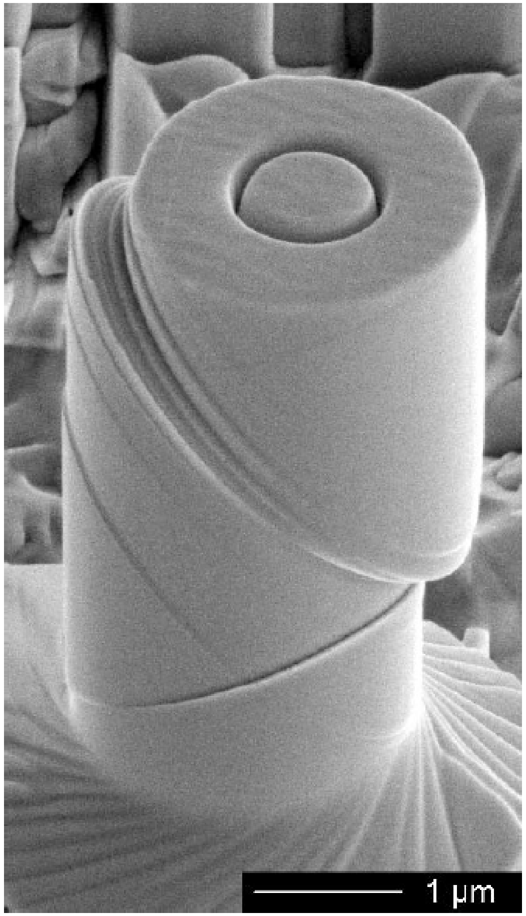
**Grain-boundary strengthening** (or **Hall–Petch strengthening**) is a method of strengthening materials by changing their average crystallite (grain) size. It is based on the observation that grain boundaries impede dislocation movement and that the number of dislocations within a grain have an effect on how easily dislocations can traverse grain boundaries and travel from grain to grain. So, by changing grain size one can influence dislocation movement and yield strength. For example, heat treatment after plastic deformation and changing the rate of solidification are ways to alter grain size.[1]



# Plastic deformation-dislocation glide

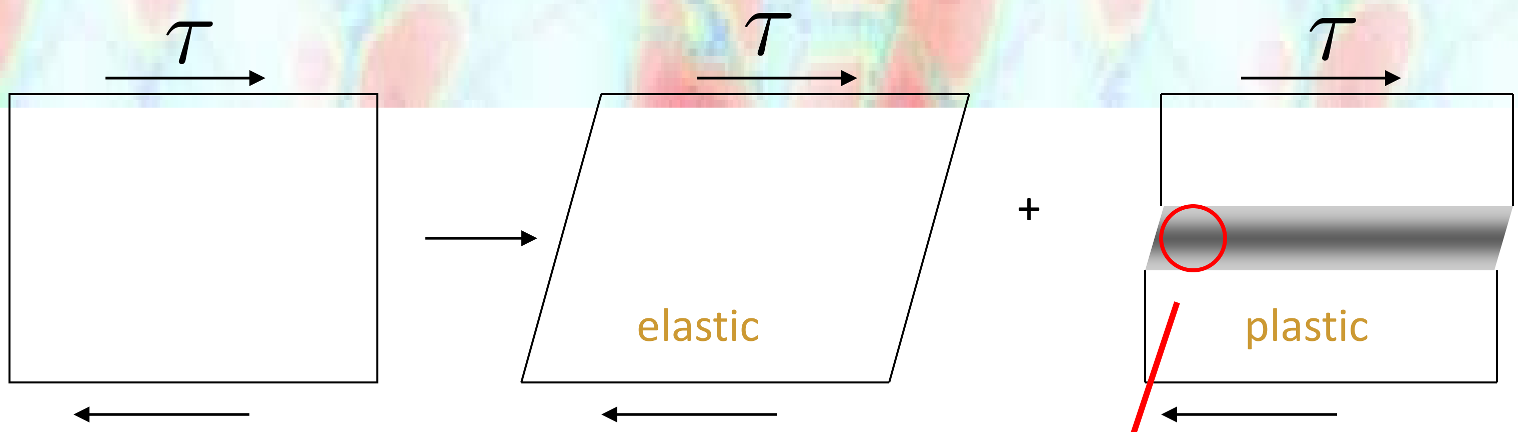


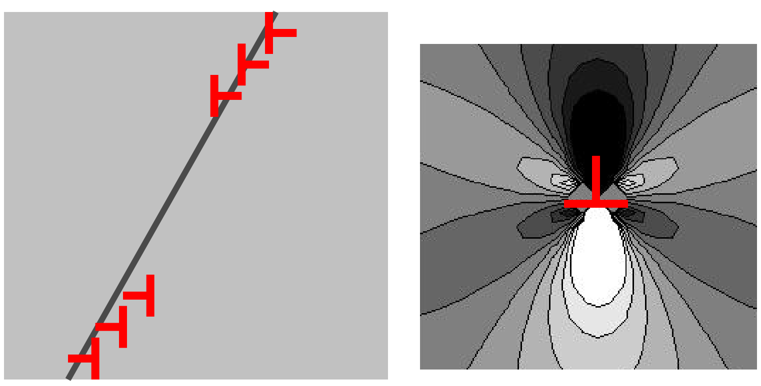




Uchic, Dimiduk, Florando & Nix, *Science*, Vol 305, 13 Aug 2004, pp. 986-989

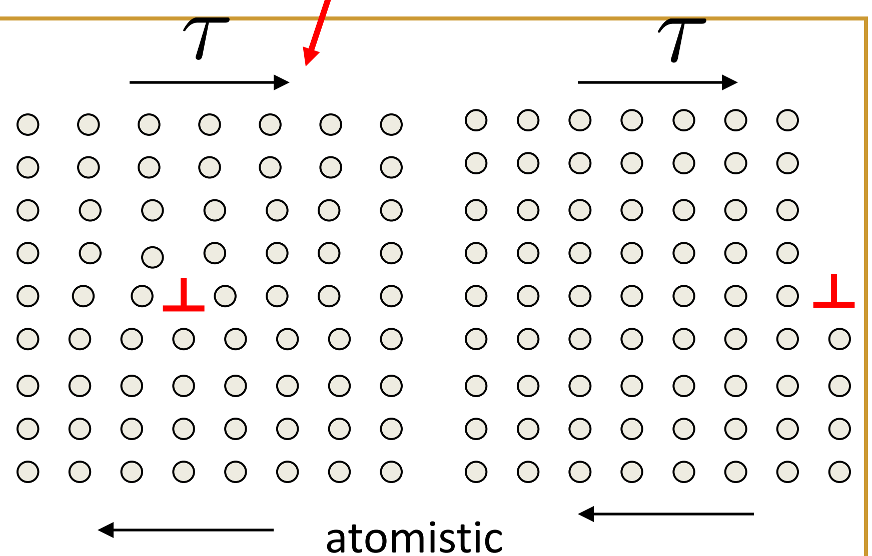
# Plastic deformation




continuum description



dislocation dynamics

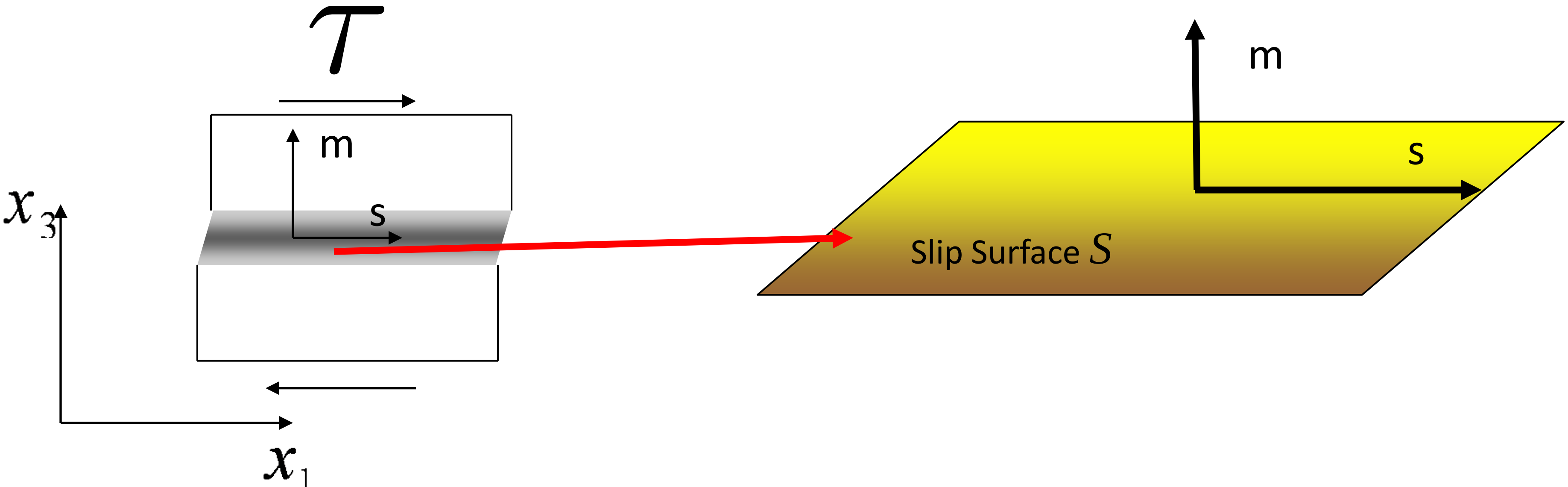



atomistic

# Micro-Macro connection

Macro

Micro




Plastic strain

Dislocation lines

$$\beta_{ij}^{p} = \sum_{\alpha} \xi^{\alpha} s_i^{\alpha} m_j^{\alpha}$$

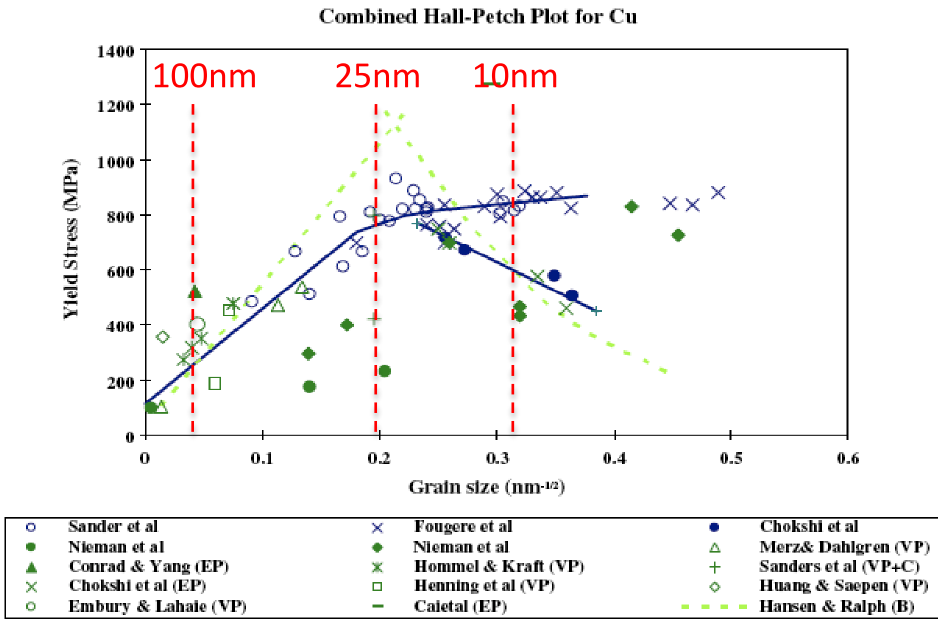
$$\alpha_{ij} = \xi_{,k} e_{ikl} s_l m_j$$

Dislocation density tensor

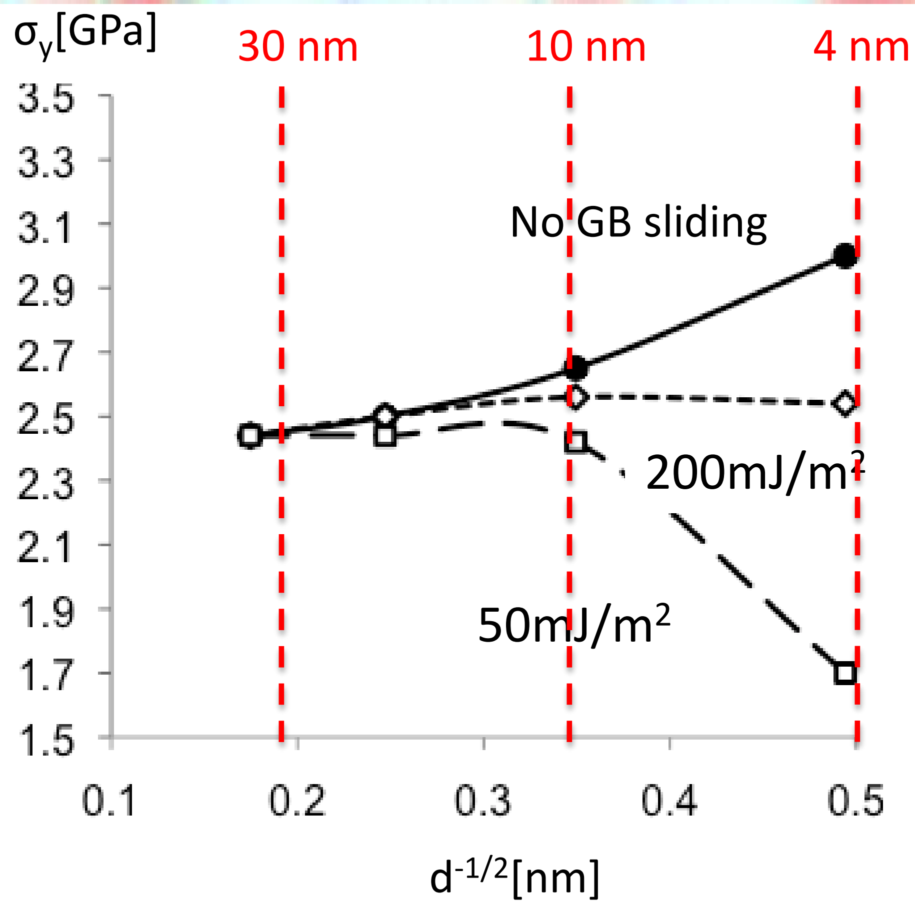
$$\alpha_{ij} = \beta^{p}{}_{lj,k} e_{ikl}$$

Kroner (1958)

# Size effects are well understood in polycrystalline materials




*M.A. Meyers et al / Progress in Materials Science 51 (2006) 427–556*

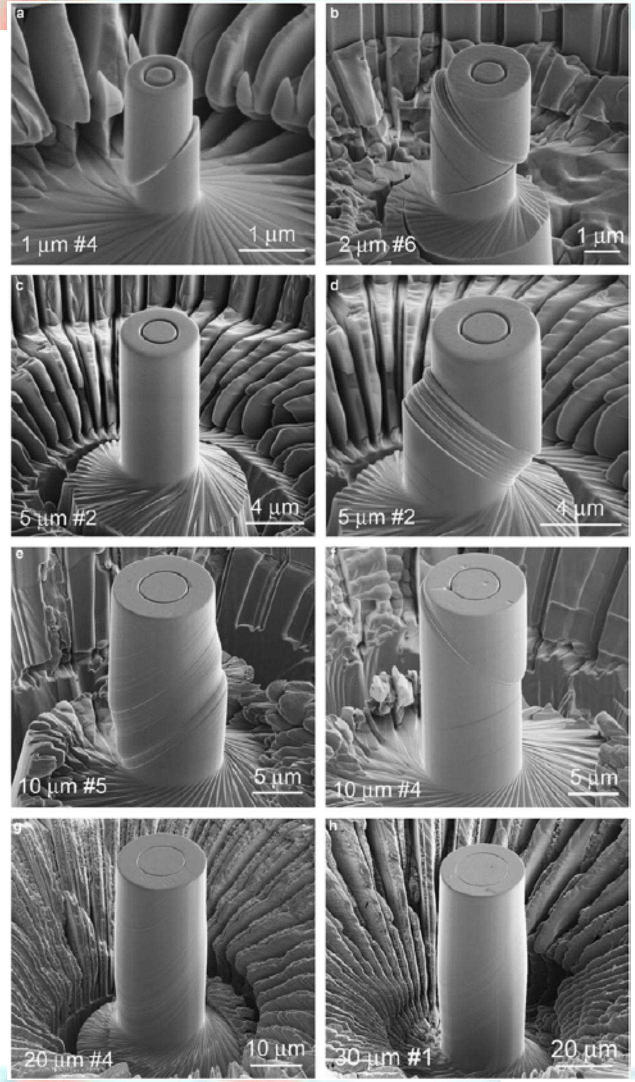


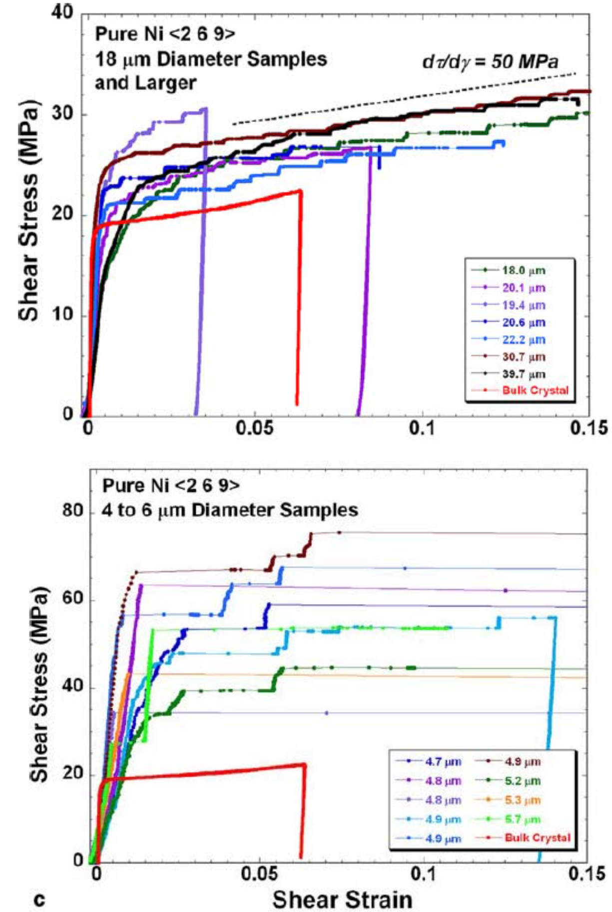

$\sigma_n = \sigma_0 + k/\sqrt{d}$ for coarse-grained metals

$\sigma_n \sim 1/d$ for nanocrystalline metals.

Koslowski, et al. JMPS 2011

# Size effects are well understood in single crystals



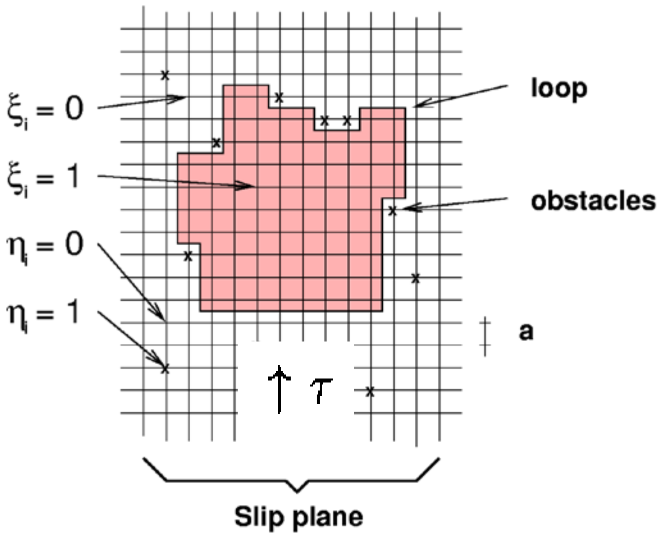




Uchic, Dimiduk, Florando & Nix, *Science*, Vol 305, 13 Aug 2004, pp. 986-989

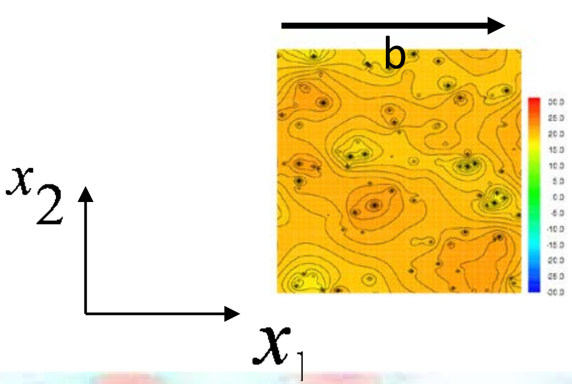
# Outline

- Phase field dislocation dynamics.
- Incorporating the stacking fault energy in dislocation dynamics
- Effect of stacking fault energy
- Size effects
- Strain rate effects

# Phase field dislocation model

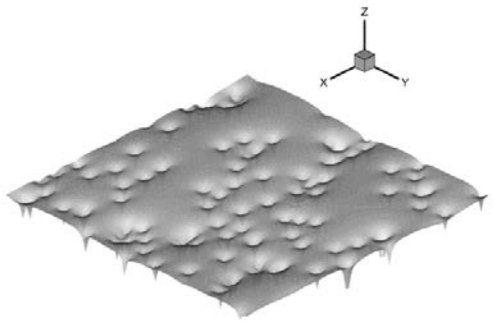



Lattice model of dislocation loop-point obstacle interaction



Scalar phase-field

$$\xi(x_1, x_2, x_3)$$

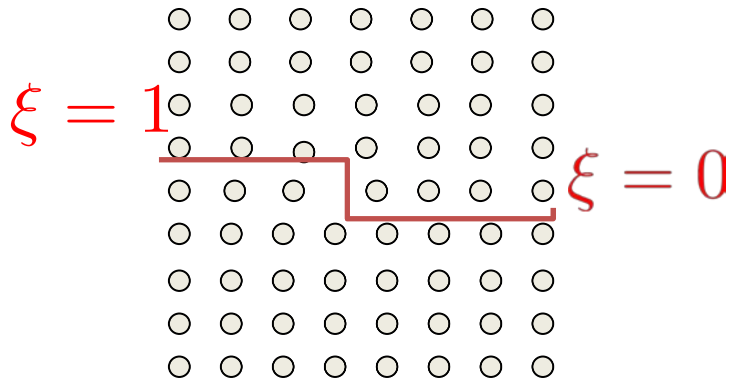


$$\alpha_{12} = \frac{\partial \xi}{\partial x_1}$$ edge dislocations

$$\alpha_{11} = -\frac{\partial \xi}{\partial x_2}$$ screw dislocations

# Phase field dislocation dynamics

$$\frac{\partial \xi(x)}{\partial t} = -L\frac{\delta E}{\delta \xi(x)}$$



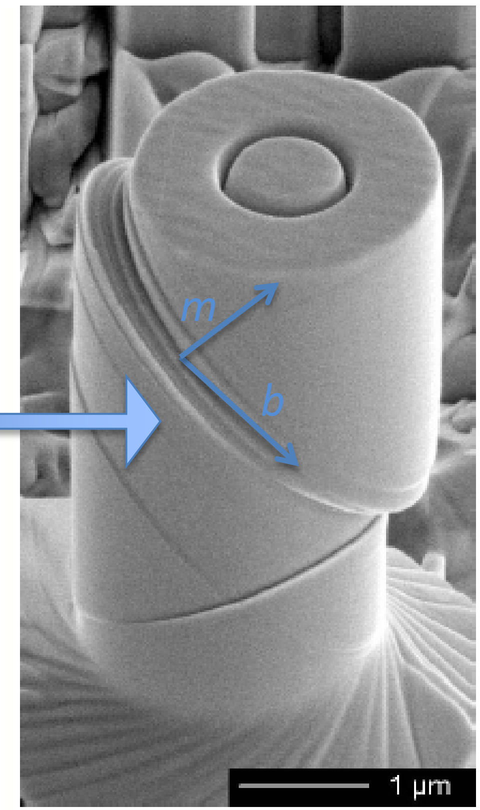

$$E = E^{int} + E^{misfit} + E^{ext}$$

$$E^{\text{int}} = \frac{1}{2}\int \hat{A}_{mnuv}(k)\hat{\beta}^{p}_{mn}(k)\hat{\beta}^{p*}_{uv}(k)\frac{d^3k}{(2\pi)^3}$$

$$\beta^{p}_{ij}(x) = \sum_{\alpha=1}^{N_s}\sum_{n_\alpha=1}^{N}\xi^{\alpha}_{n_\alpha}(x)\delta_{n_\alpha}m^{\alpha}_{i}b^{\alpha}_{j}$$

$$\hat{A}_{mnuv}(k) = c_{mnuv} - c_{kluv}c_{ijmn}\hat{G}_{ki}(k)k_jk_l$$

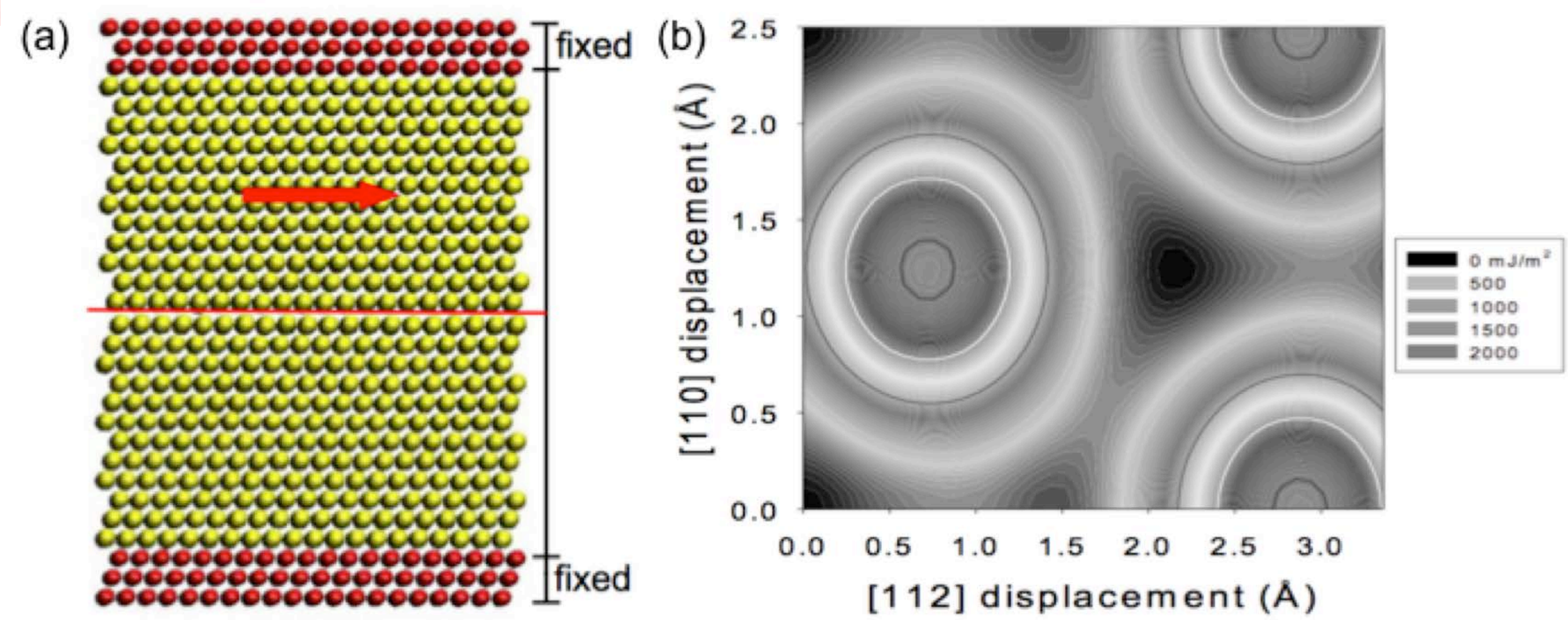
$$G_{ij}(\boldsymbol{r}-\boldsymbol{r}') = \frac{1}{4\pi\mu}\frac{\delta_{ij}}{|\boldsymbol{r}-\boldsymbol{r}'|} - \frac{1}{16\pi\mu(1-\nu)}\frac{\partial^2}{\partial r_i \partial r_j}|\boldsymbol{r}-\boldsymbol{r}'|$$




SEM images of pure Ni micro-crystals (Uchic, Science 2004)

Koslowski, Cuitino and Ortiz, JMPS (2002)
Hunter, Le, Saied and Koslowski, Journal High Performance Computing (2011), Cao and Koslowski Acta Materialia (2013)

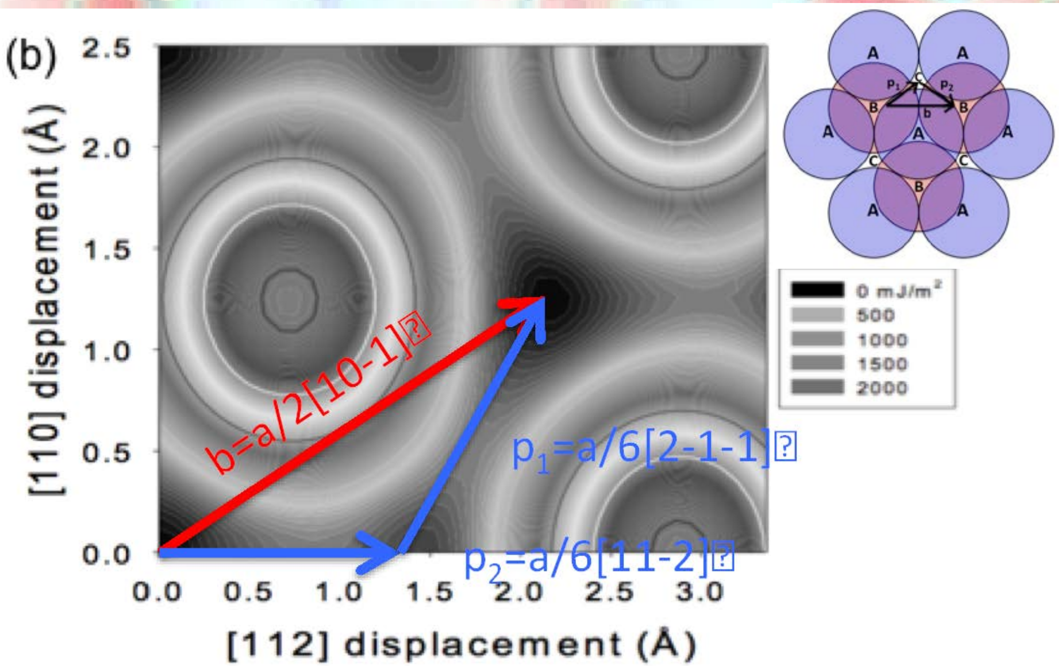
# Stacking fault energy

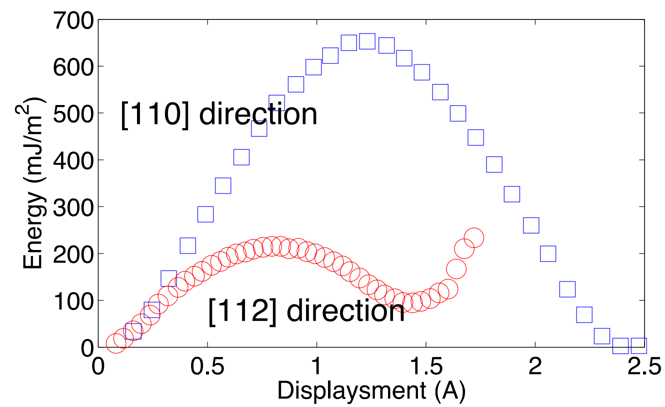



$$E^{misfit} = \sum_{\alpha=1}^{N_s} \sum_{n_\alpha=1}^{N} \int \phi_{n_\alpha}(x) d^3x$$

Lee, Kim, Strachan and Koslowski PRB (2010)
Hunter, Beyerlein, Germann, Koslowski, PRB (2011)

# Stacking fault energy

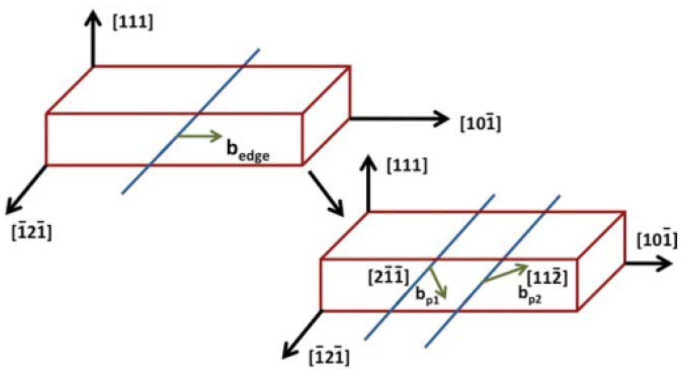



$$
\begin{aligned}
\phi(\xi_1,\xi_2,\xi_3) = \{ & c_0 + c_1[\cos 2\pi(\xi_1-\xi_2) + \cos 2\pi(\xi_2-\xi_3) + \cos 2\pi(\xi_3-\xi_1)] \\
& + c_2[\cos 2\pi(2\xi_1-\xi_2-\xi_3) + \cos 2\pi(2\xi_2-\xi_3-\xi_1) + \cos 2\pi(2\xi_3-\xi_1-\xi_2)] \\
& + c_3[\cos 4\pi(\xi_1-\xi_2) + \cos 4\pi(\xi_2-\xi_3) + \cos 4\pi(\xi_3-\xi_1)] \\
& + c_4[\cos 4\pi(3\xi_1-\xi_2-2\xi_3) + \cos 4\pi(3\xi_1-2\xi_3-\xi_3) + \cos 4\pi(3\xi_2-\xi_3-2\xi_1) \\
& + \cos 4\pi(3\xi_2-2\xi_3-\xi_1) + \cos 4\pi(3\xi_3-\xi_1-2\xi_2) + \cos 4\pi(3\xi_3-2\xi_1-\xi_2)] \\
& + a_1[\sin 2\pi(\xi_1-\xi_2) + \sin 2\pi(\xi_2-\xi_3) + \sin 2\pi(\xi_3-\xi_1)] \\
& + a_3[\sin 4\pi(\xi_1-\xi_2) + \sin 4\pi(\xi_2-\xi_3) + \sin 4\pi(\xi_3-\xi_1)]\}
\end{aligned}
$$

Lee, Kim, Strachan and Koslowski PRB (2010)
Hunter, Beyerlein, Germann, Koslowski, PRB (2011)

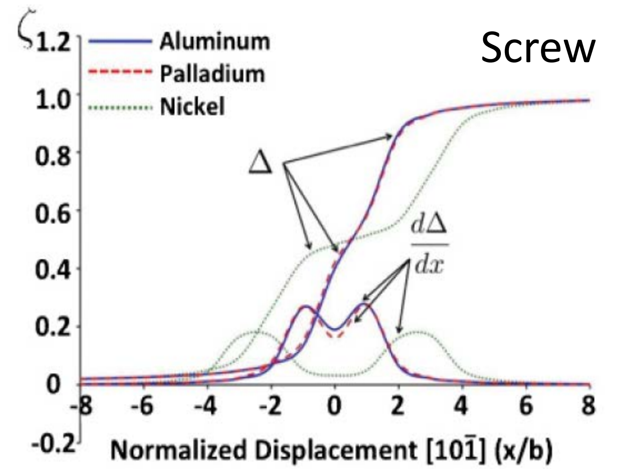
# Equilibrium stacking fault distance

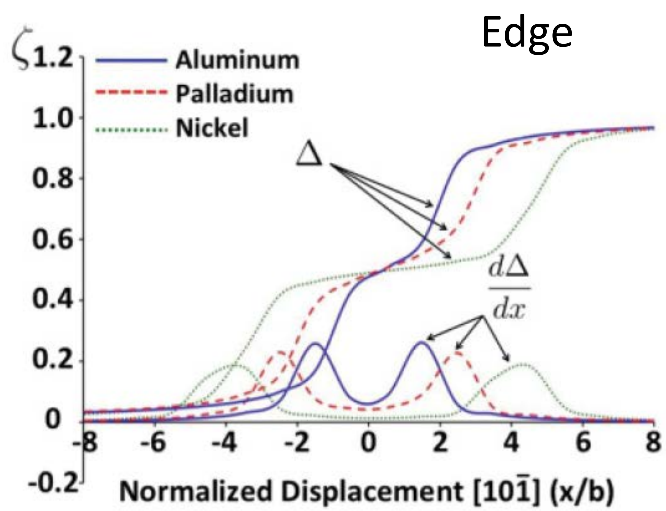



| Material | $\gamma_I(\frac{mJ}{m^2})$ | $\gamma_U(\frac{mJ}{m^2})$ | $\mu$(GPa) | $E$(GPa) | $a$(Å) | $b$(nm) |
|---|---|---|---|---|---|---|
| Aluminum | 141.78 | 172.3 | 26.50 | 70.0 | 4.05 | 0.286 |
| Palladium | 177.82 | 255.80 | 53.2 | 144.0 | 3.89 | 0.275 |
| Nickel | 84.72 | 211.69 | 75.0 | 200.0 | 3.52 | 0.249 |

| Material | Orientation | $R_e$ (b) [Eq. (17)] | $R_e$ (b) [Eq. (10)] |
|---|---|---|---|
| Aluminum | edge | 2.54 | $3.0 \pm 0.5$ |
| Aluminum | screw | 1.04 | $1.8 \pm 0.5$ |
| Palladium | edge | 4.15 | $4.9 \pm 0.5$ |
| Palladium | screw | 1.54 | $1.8 \pm 0.5$ |
| Nickel | edge | 8.04 | $8.1 \pm 0.5$ |
| Nickel | screw | 5.11 | $5.2 \pm 0.5$ |

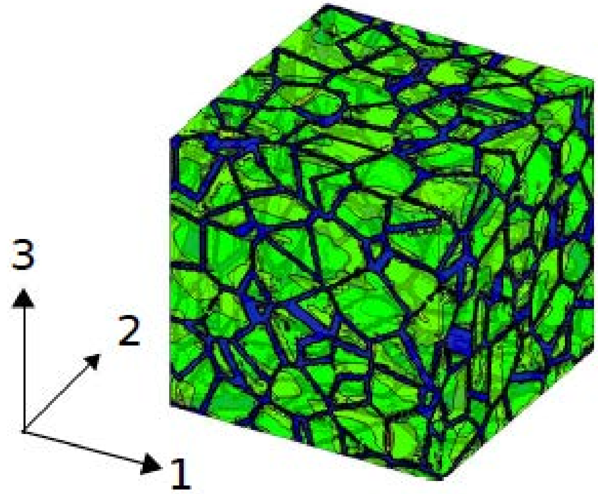
$$R_e = \frac{\mu}{2\pi\gamma_I}\left[(\boldsymbol{b}_2 \cdot \boldsymbol{\xi}_2)(\boldsymbol{b}_3 \cdot \boldsymbol{\xi}_3) + \frac{(\boldsymbol{b}_2 \times \boldsymbol{\xi}_2) \cdot (\boldsymbol{b}_3 \times \boldsymbol{\xi}_3)}{1-\nu}\right], \quad (17)$$

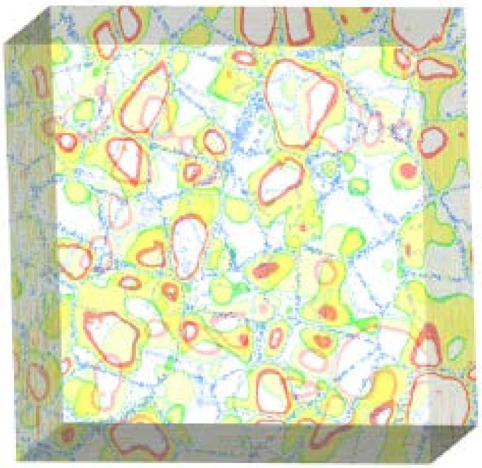



Hunter, et al. 2011

# Grain structure

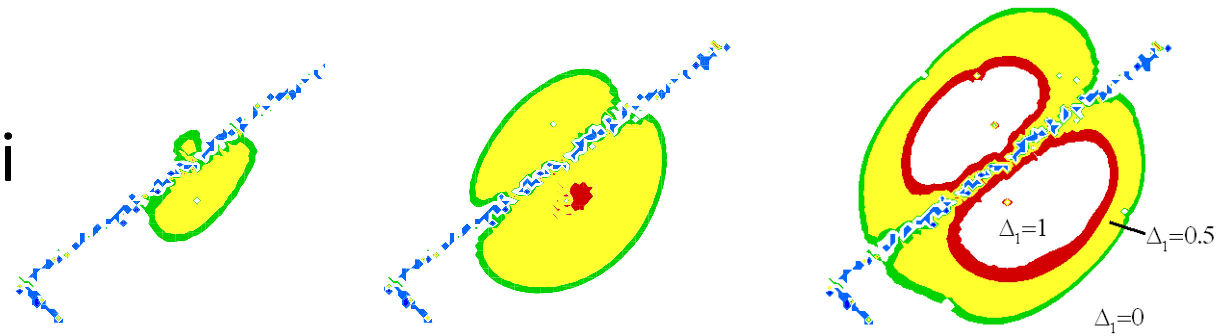


| | $\mu$ (GPa) | $E$ (GPa) | $\gamma_{sf}(\frac{mJ}{m^2})$ | $\gamma_{usf}(\frac{mJ}{m^2})$ | $a$ (nm) | $b$ (nm) | $b_p$ (nm) |
|---|---|---|---|---|---|---|---|
| Al | 26.0 | 70.0 | 141.78 | 172.3 | 0.405 | 0.286 | 0.165 |
| Ni | 75.0 | 200.0 | 84.72 | 211.69 | 0.352 | 0.249 | 0.144 |

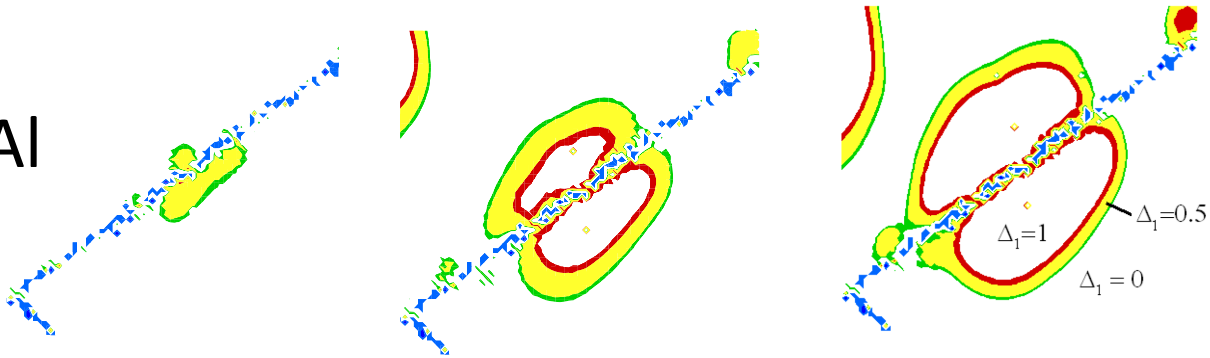
# $\gamma$ surface effects: dislocation structures

Ni



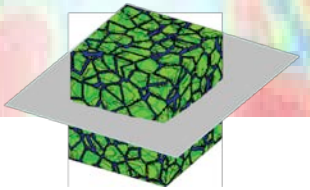

$$\gamma_I = 84mJ/m^2$$
$$\gamma_U = 211mJ/m^2$$

Al

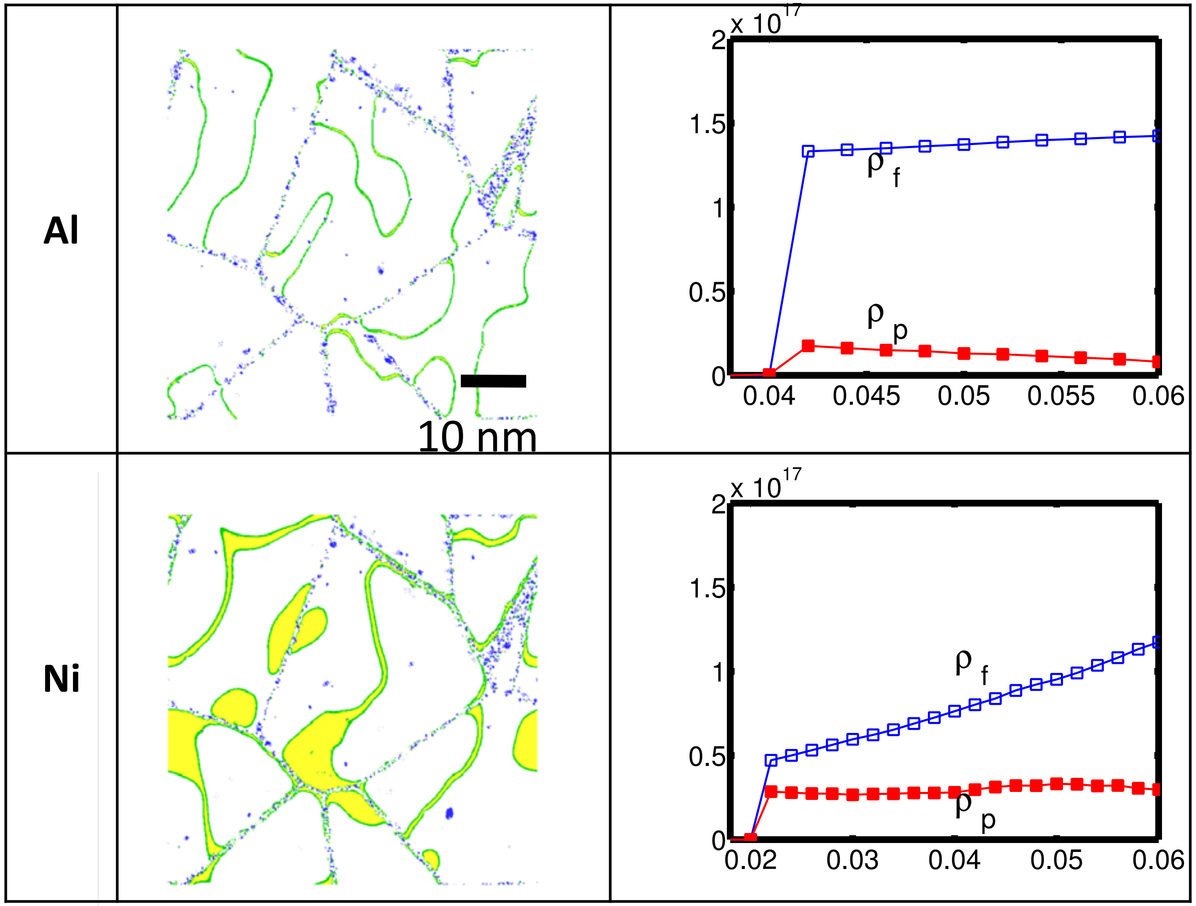



$$\gamma_I = 142mJ/m^2$$
$$\gamma_U = 172mJ/m^2$$

# $\gamma$ Surface effects: dislocation structures

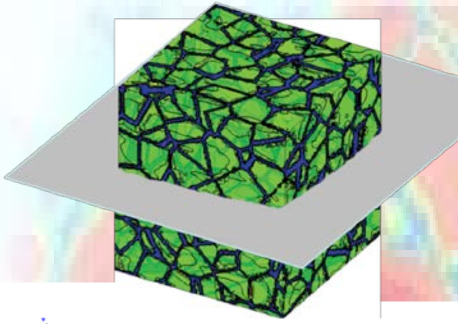


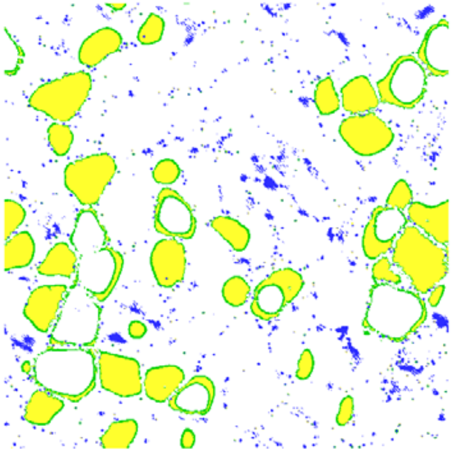
- Al has higher $\gamma_{sf}/\mu b$



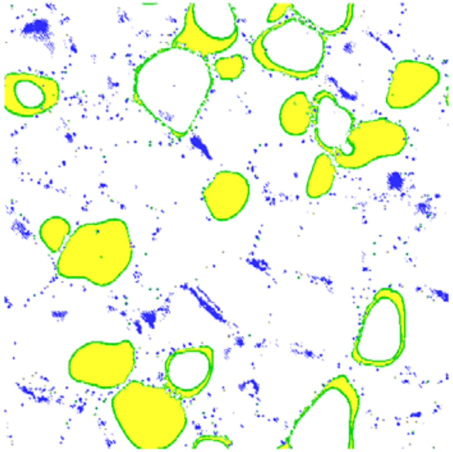

L. Cao et al., submitted to J. Mech. Phys. Solids (2014)

# Grain size

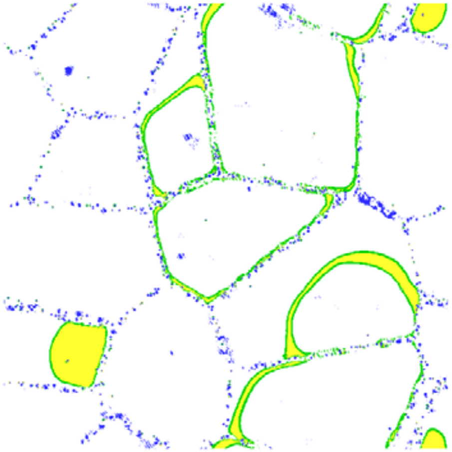




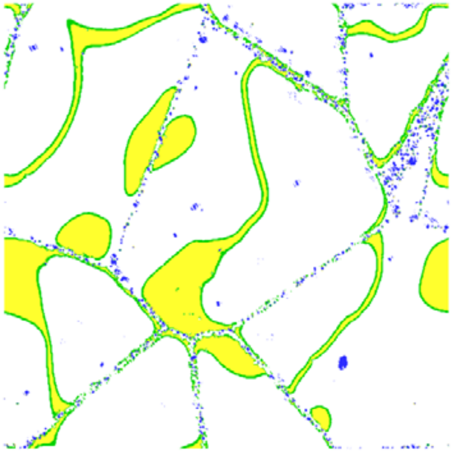
10 nm



15 nm

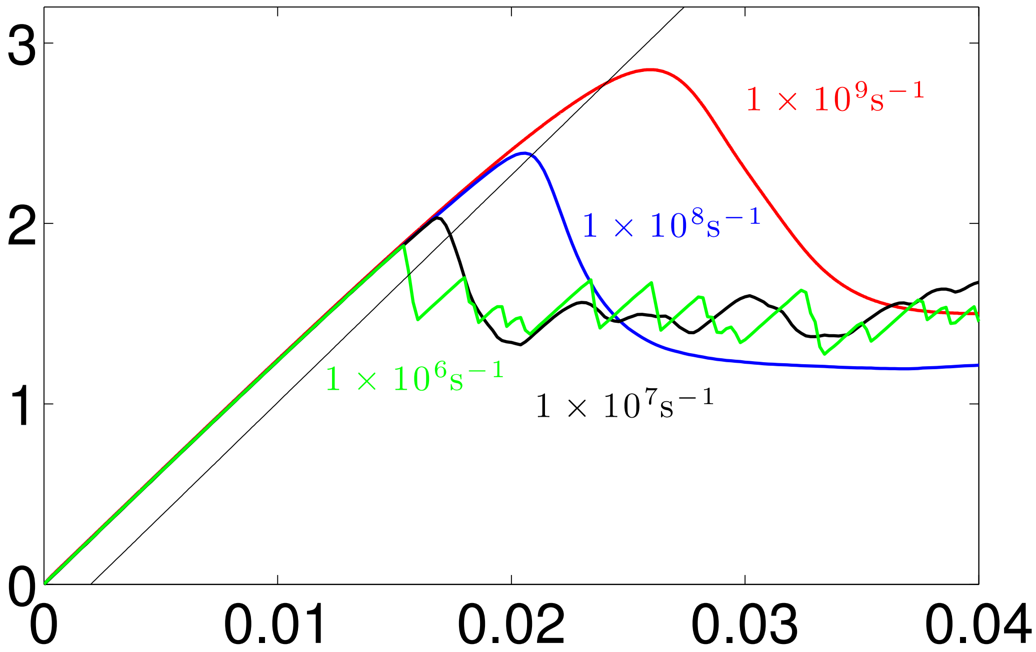


30 nm



40 nm

# Strain rate sensitivity



# Dislocation evolution: strain rate

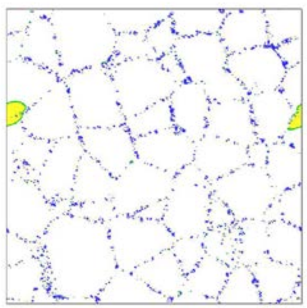
$\dot{\epsilon} = 8 \cdot 10^4 / sec$

$\dot{\epsilon} = 1.6 \cdot 10^6 / sec$

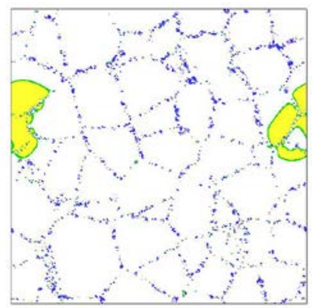
# Dislocation evolution

$$\dot{\varepsilon} = 1 \cdot 10^{6} s^{-1}$$

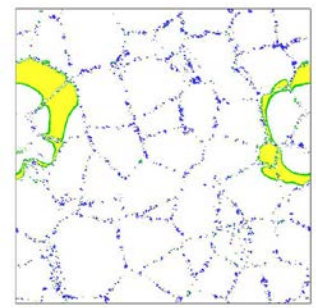
ε = 2%



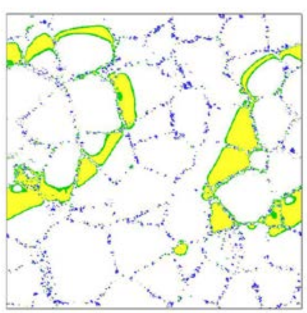
ε = 2.2%



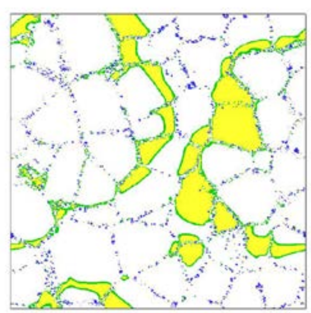
ε = 2.24%



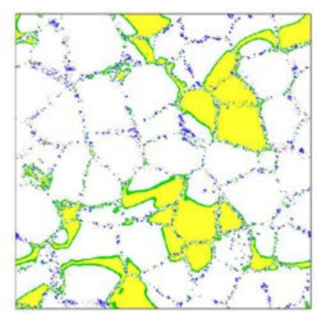
ε = 2.32%



ε = 2.36%



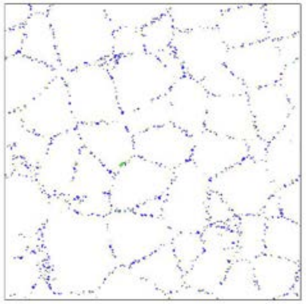
ε = 2.38%



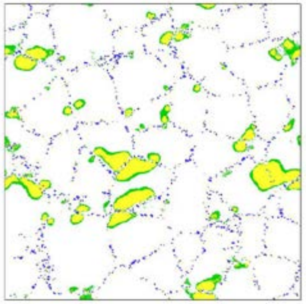
# Dislocation evolution

$$\dot{\varepsilon} = 1 \cdot 10^{8}\, s^{-1}$$

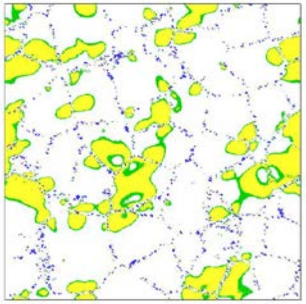
ε = 2%



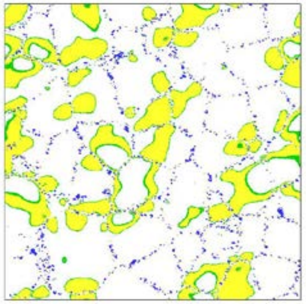
ε = 2.6%



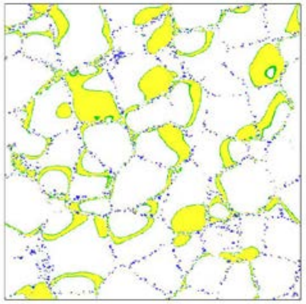
ε = 2.8%



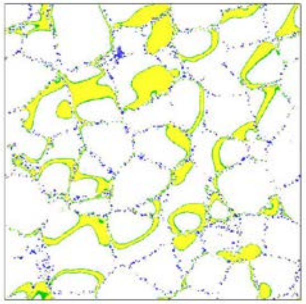
ε = 3%



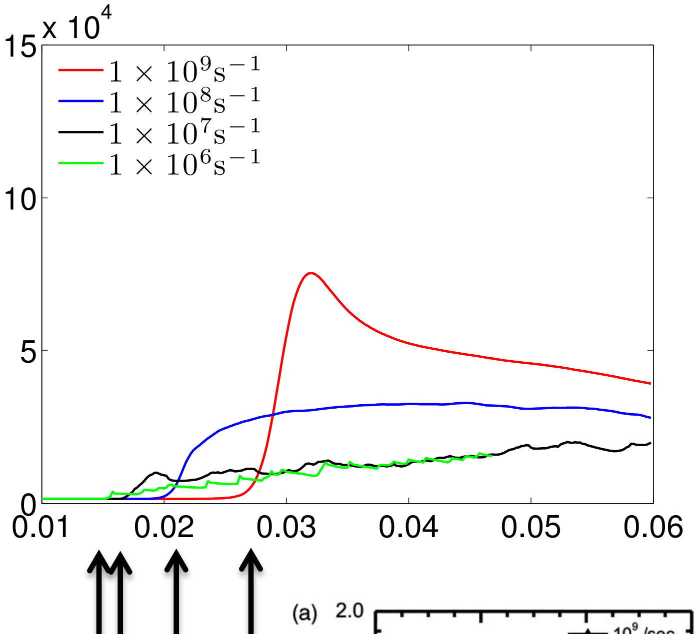
ε = 5%

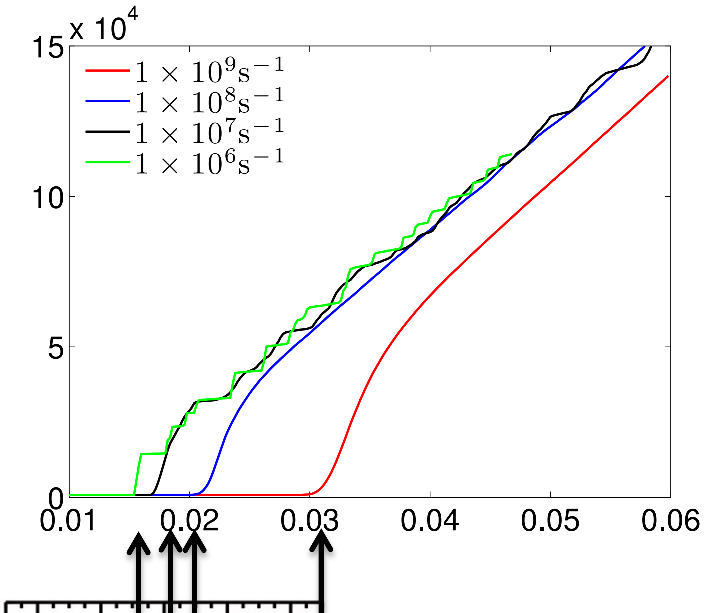


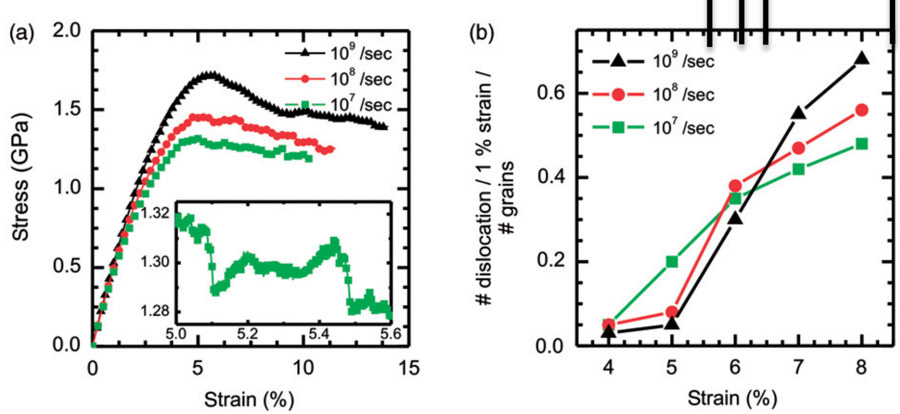
ε = 6%



# Effect of strain rate on dislocation density

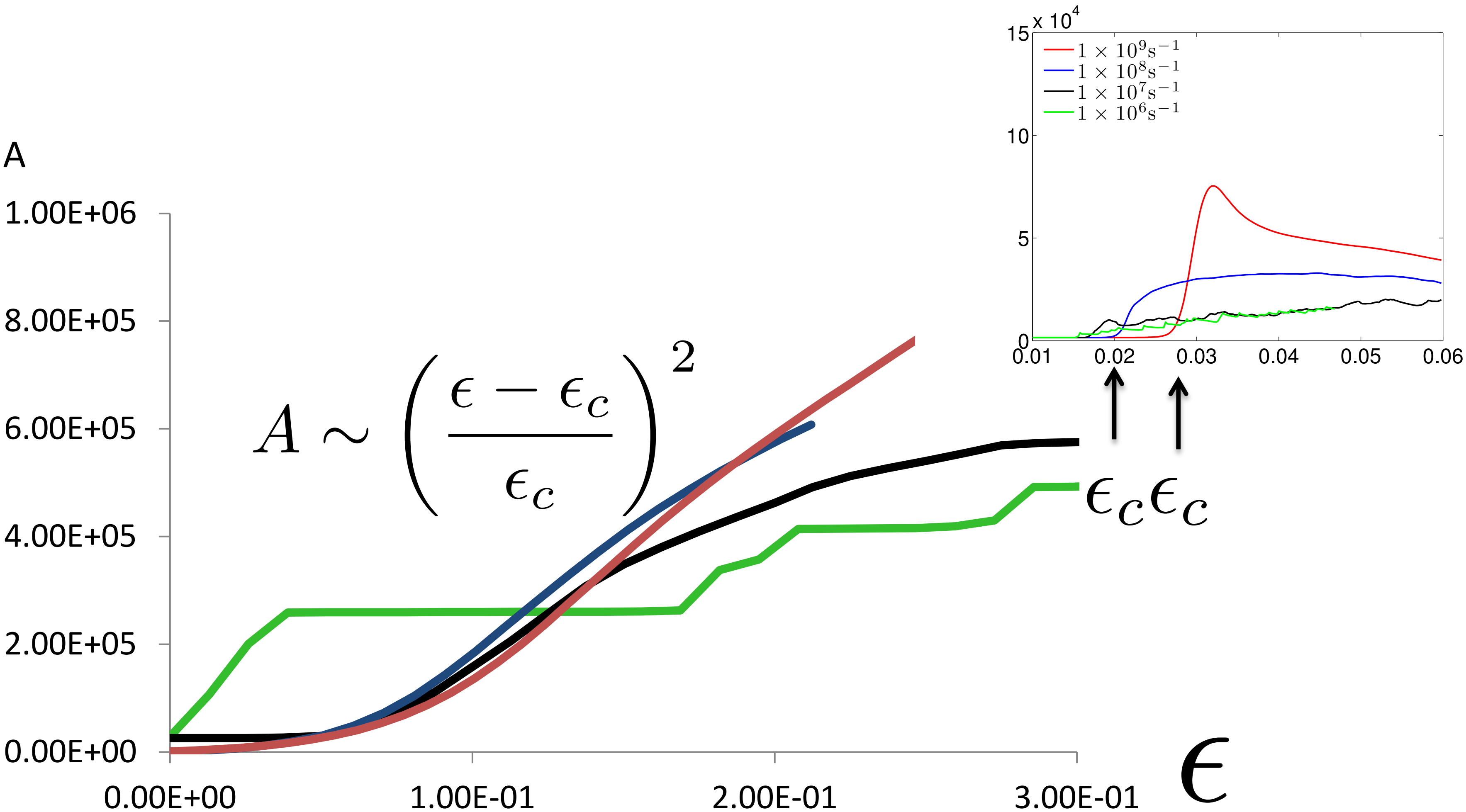



Brandl et al. Philos. Mag. (2009)

PURDUE UNIVERSITY

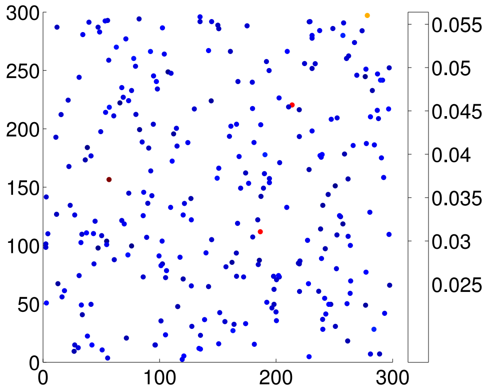


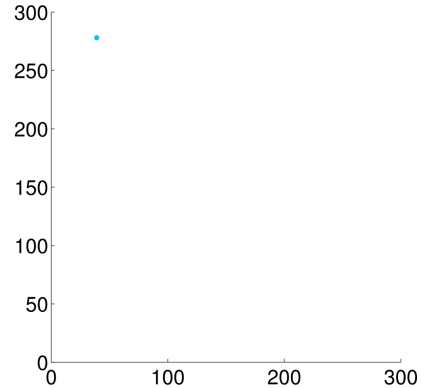

$$A \sim \left( \frac{\epsilon - \epsilon_c}{\epsilon_c} \right)^2$$

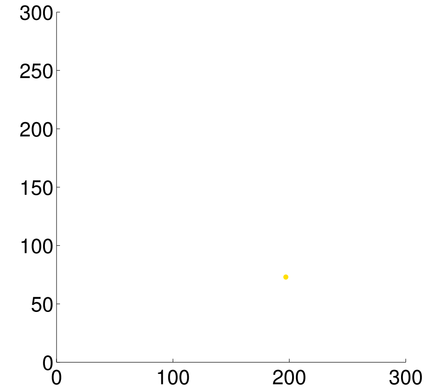
# Dislocation evolution

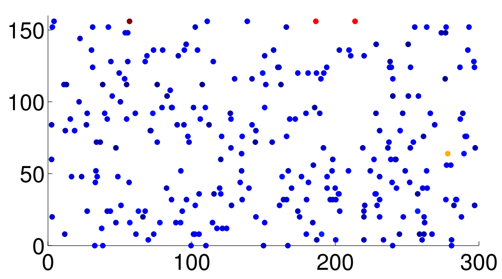
# Nucleation rate

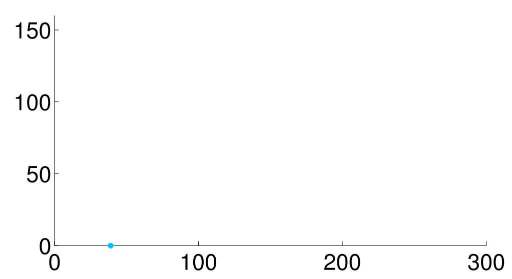
$\dot{\varepsilon} = 10^8\ /\ \mathrm{sec}$ $\dot{\varepsilon} = 10^7\ /\ \mathrm{sec}$ $\dot{\varepsilon} = 10^6\ /\ \mathrm{sec}$

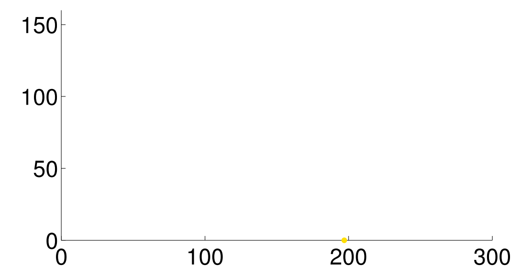


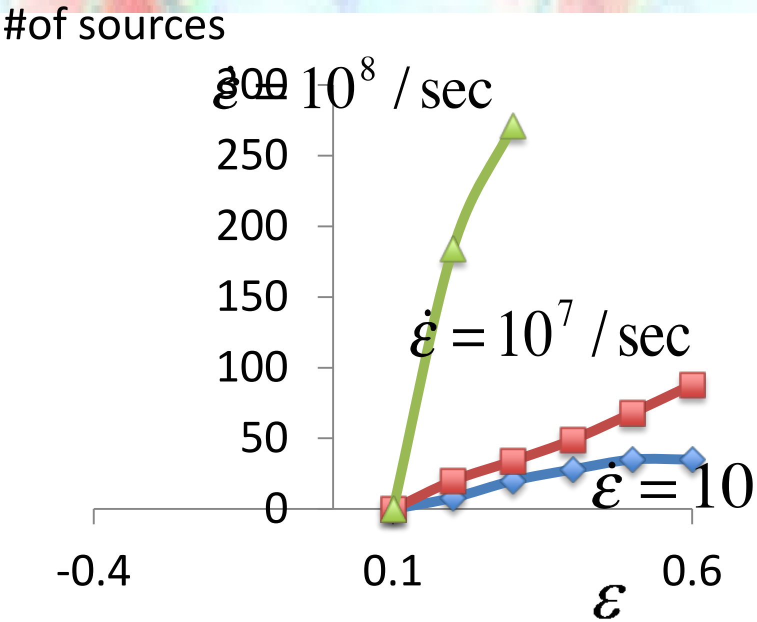



# Transition State Theory




The first nucleation probability distribution is

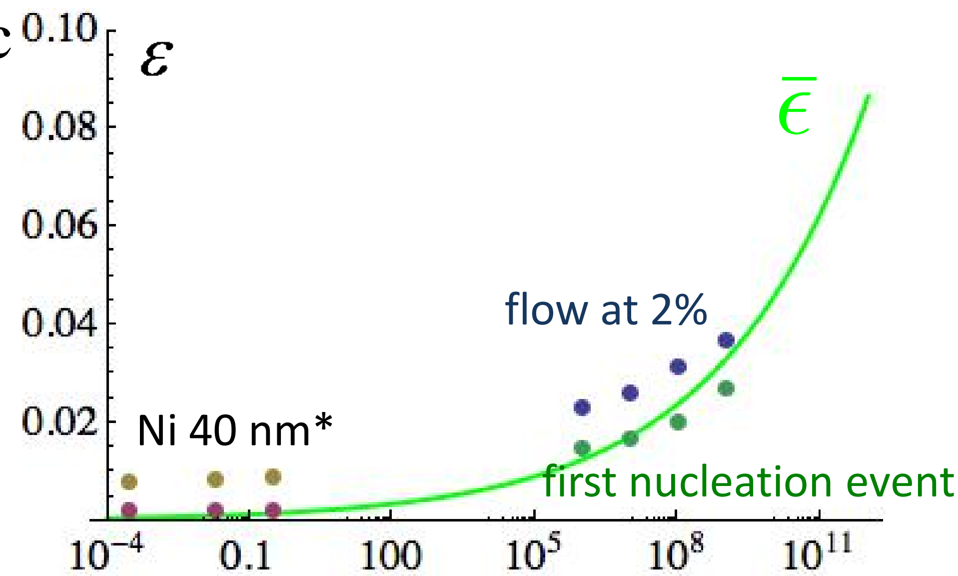
$$p(\varepsilon) = \frac{1}{C\dot{\varepsilon}} k(\varepsilon) e^{-\frac{1}{\dot{\varepsilon}}\int_0^{\varepsilon} k(\varepsilon') d\varepsilon'}$$

$$\bar{\varepsilon} = \int_0^{\varepsilon_c} \varepsilon \, p(\varepsilon) d\varepsilon$$

The nucleation rate is:

$$k(\varepsilon) = k_0 A(\dot{\varepsilon})\varepsilon$$

$$A(\dot{\varepsilon}) = 0.004\dot{\varepsilon}^{0.7}$$




*(Schwaiger et al., 2003) values are multiplied by 0.1 and 0.4 to obtain the CRSS

# Summary

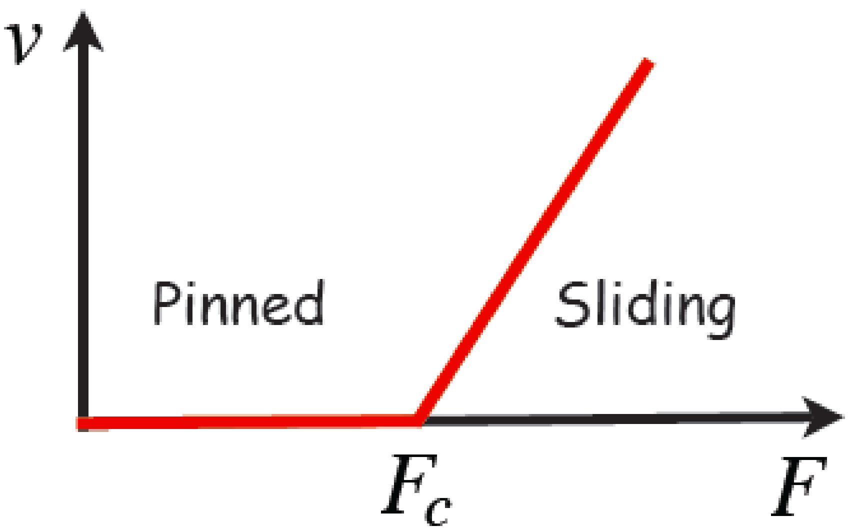
- We study effects of microstructure and strain rate on the deformation mechanisms of nanocrystalline Ni.
- Predictions:
  - Hall-Petch effect
  - Inverse Hall-Petch effect depends on the GB energy.
  - Stacking fault width and density of partial dislocation depend on USF and ISF.
  - Strain rate plays an important role on deformation mechanisms: high strain rate increases density of partial dislocations and delays the onset of nucleation.
  - TST can be used to obtain flow rules at strain rates $10^0$/sec to $10^5$/sec

Acknowledgements:
DOE-BES

Collaborators: H. Kim, A. Strachan, Purdue University
I. J. Beyerlein, A. Hunter, LANL

# Universality, self-similarity and scaling

Because dislocation-driven plastic flow exhibit a scale-free behavior over many decades of sizes, its properties are independent of microscopic and macroscopic details, and great progress can be made by the use of simple models.



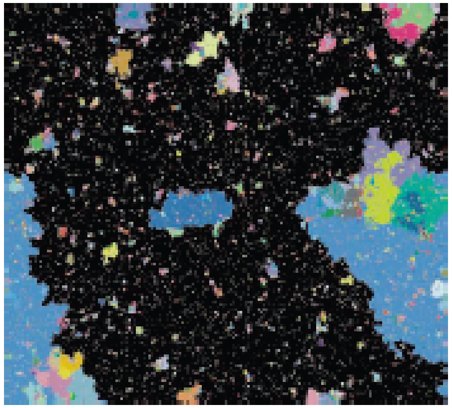

$$\frac{\partial \xi(x)}{\partial t} = K[\xi(x)] + \tau - \eta(x, \xi(x))$$

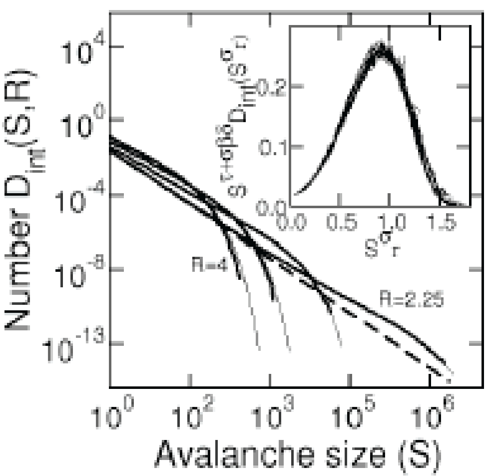
Non-local kernel

Pinning potential

# Avalanches-SOC

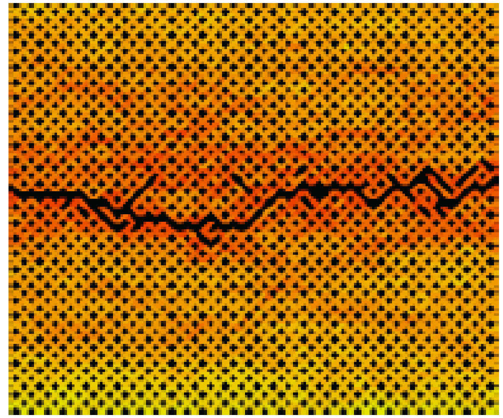
## Magnetism

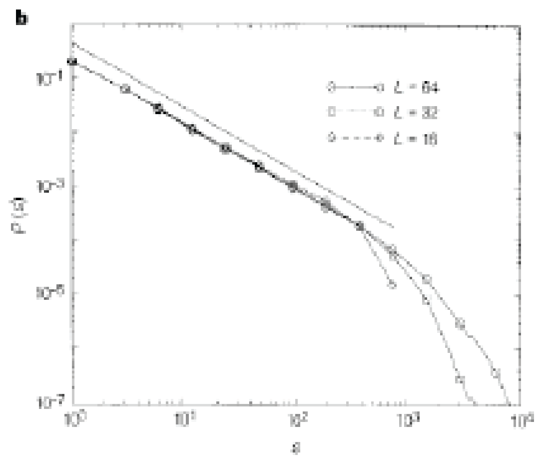





Sethna, JP; Dahmen, KA; Myers, CR.
Nature, 2001.

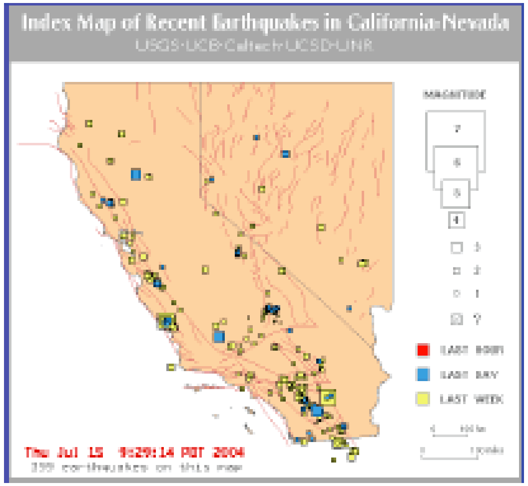
## Fracture

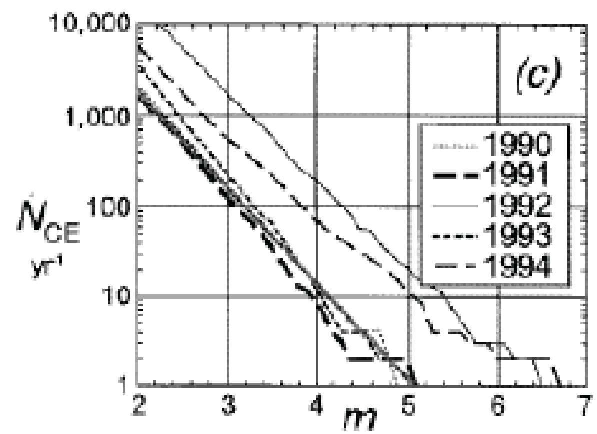





Zapperi, S:Vespignani, A: Stanley, HE.
Nature, 1997.

## Earthquakes

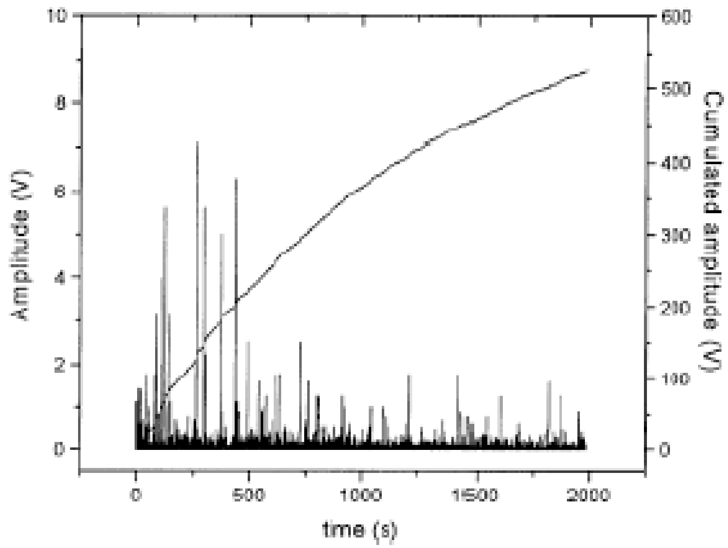


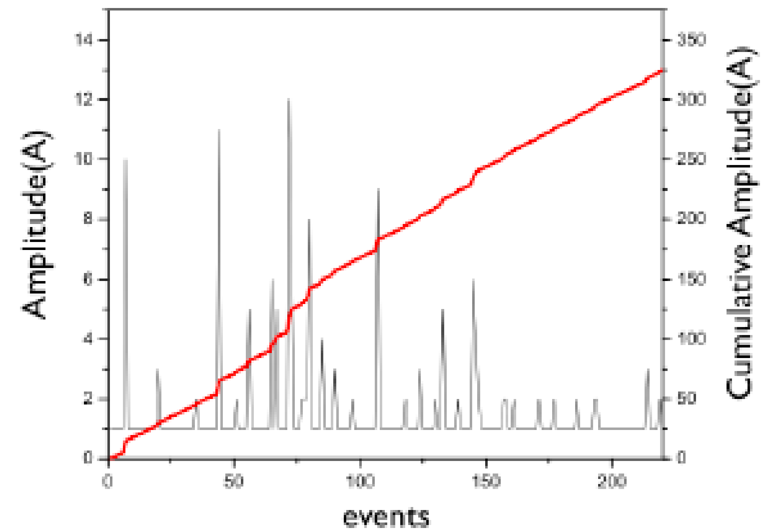

Tucotte, DL.
Rep. Prog. Phys, 1999.

# Intermittent dislocation flow in plastic deformation

- The AE signal accompanying the plastic deformation consists of many overlapping pulses as observed experimentally in metallic single crystals (Vinogradov, 2001) and ice single crystals (Weiss, 1997).
- The instantaneous dissipation shows burst of activity that can be considered as dislocation avalanches.
- The cumulated activity is a measure of the strain and and also shows the burst character observed in plastic deformation.(Pond,1973 and Neuhauser, 1983)




Instantaneous and cumulated acoustic activity during a loading step in a compression test (Weiss, 1997).

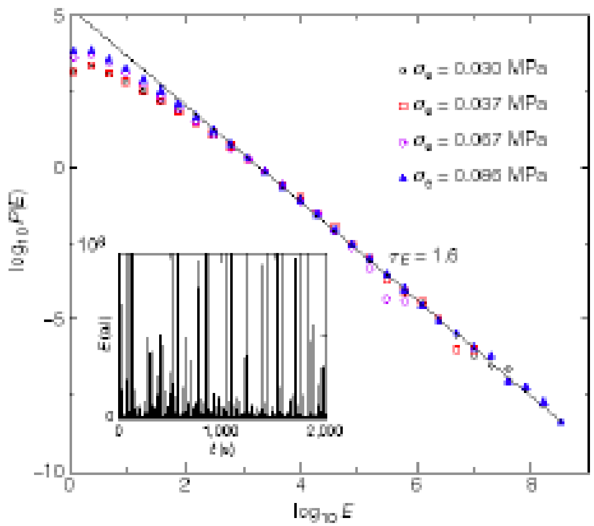



Predicted acoustic activity during a loading step (Koslowski, 2004).

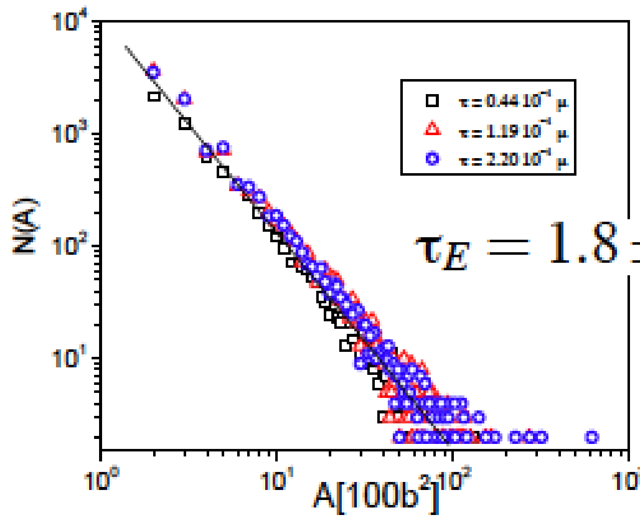
# Scale-free dislocation avalanches

- Recently, acoustic emission experiments on single crystals of ice showed an intermittent and heterogeneous plastic flow.
- The probability density function of the energy, follows a power law distribution

$$P(E) \sim E^{-\tau_E}$$




Statistical properties of acoustic energy bursts under constant stress (Miguel, 2001)

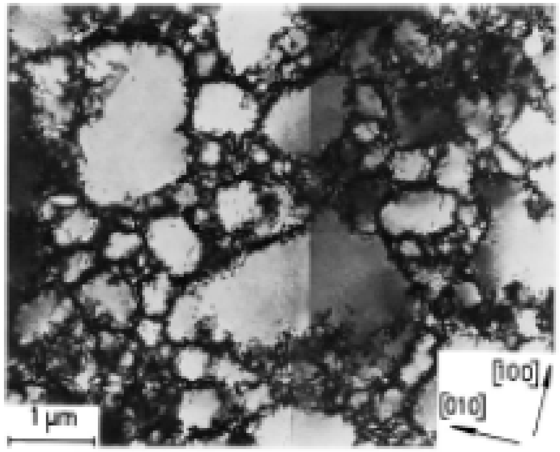



$$\tau_E = 1.8 \pm 0.1$$

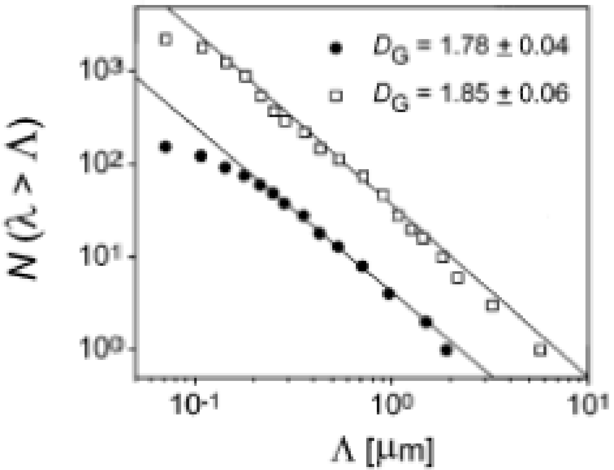
Simulated acoustic energy bursts under constant stress

Koslowski, et al. PRL 2004.

# Characterization of self-similar cell structures




TEM micrograph of dislocation cells of single copper deformed at 75.6MPa (Mughrabi, et.al. 1986)




Cell distribution for deformed single crystal of copper and determination of the fractal dimension (Hahner, et.al. 1998).

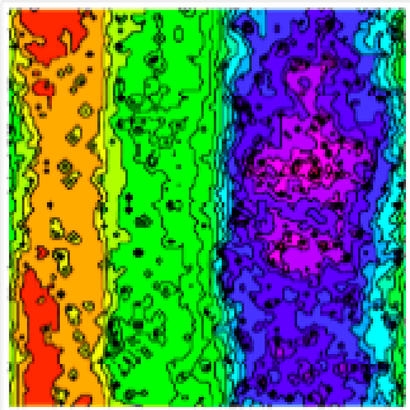
# Characterization of self-similar cell structures

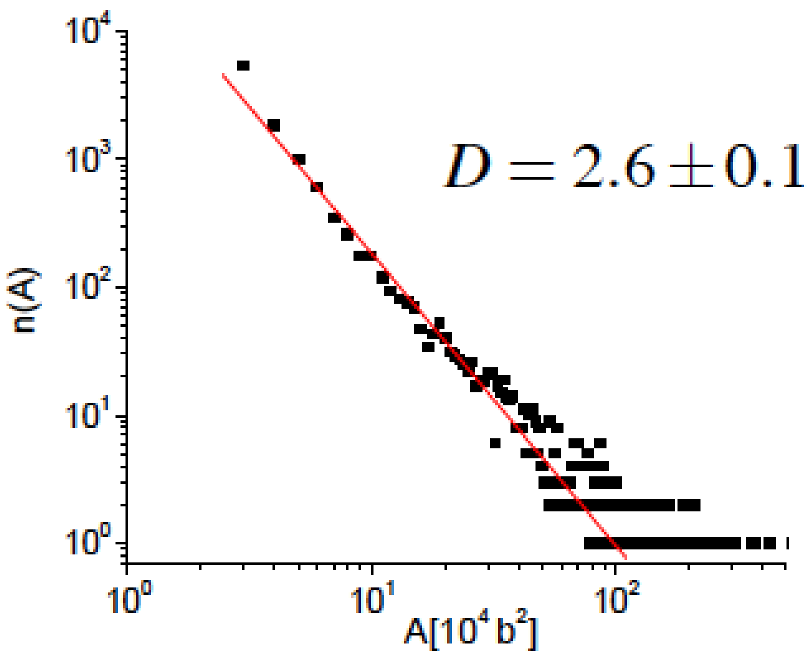
The cell size distribution has an hyperbolic frequency:

$$n(A) = CA^{-D}$$

Formation of cell structures corresponds to the regimen

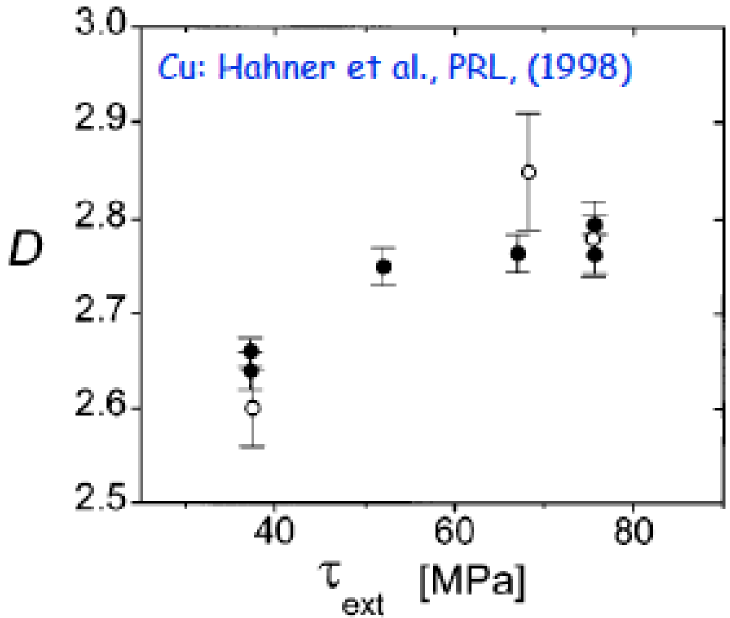
$$2 < D < 3$$

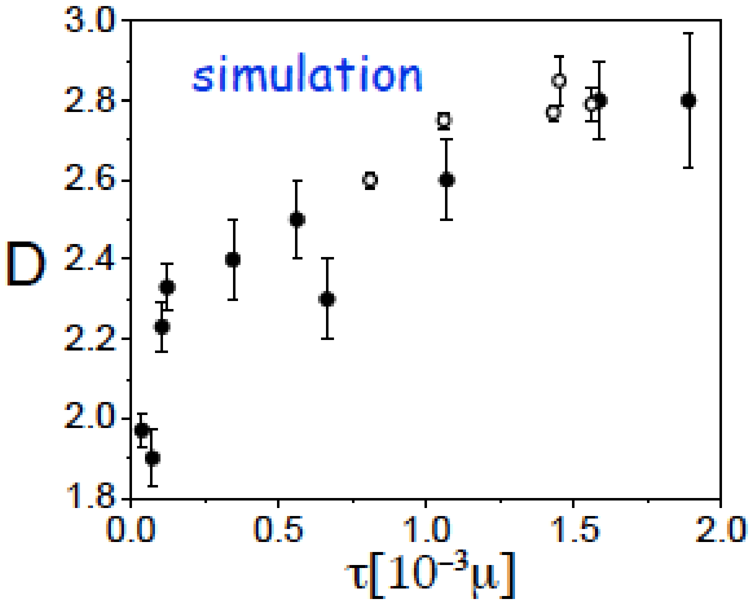





applied stress: $\tau = 1.1 \cdot 10^{-3} \mu$

# Fractal exponent



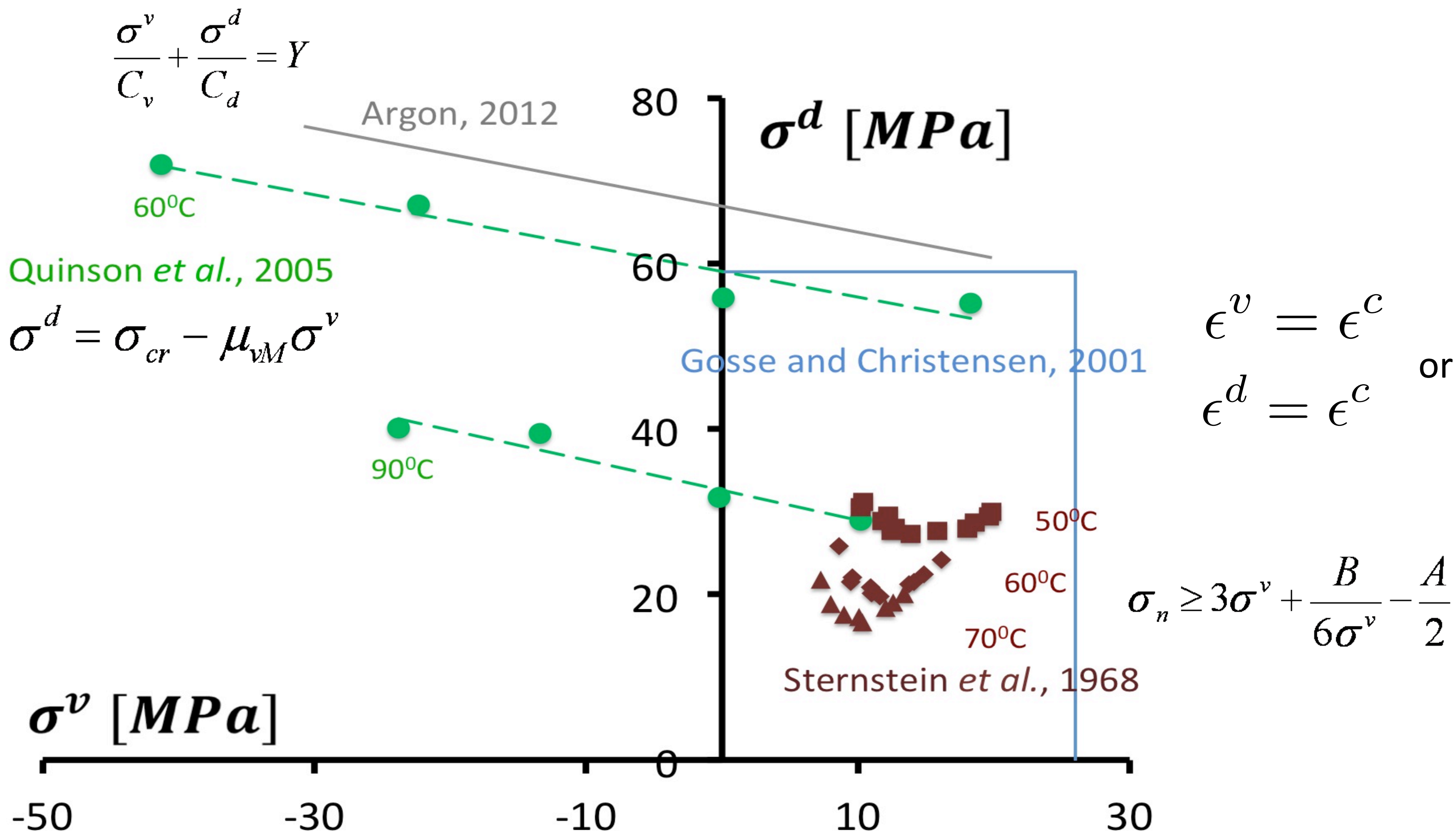




The 2D model shows excellent agreement with experiment, from stress-strain to density to fractal dimension of structures.

# *Local failure criterion for crazing and shear in amorphous polymers*

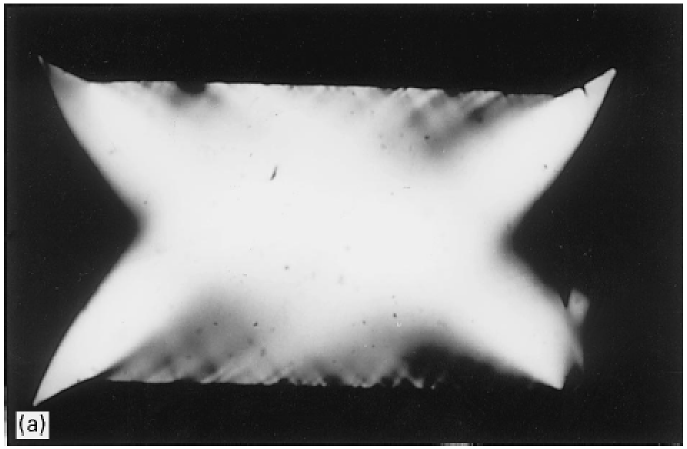
*Marisol Koslowski*
School of Mechanical Engineering
Purdue University

# Experimental data

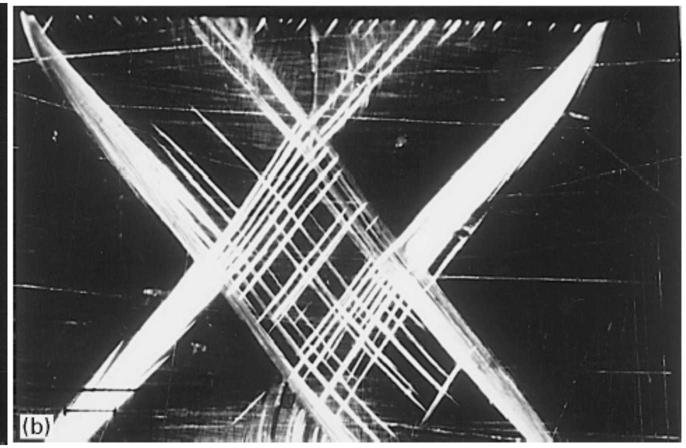



Data collected from experimental literature showing volumetric versus deviatoric stress at failure

# Damage in amorphous polymers

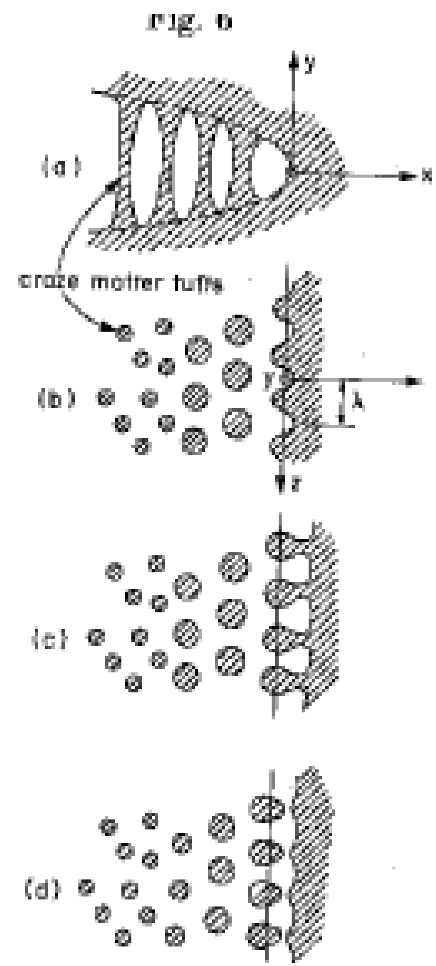



PMMA

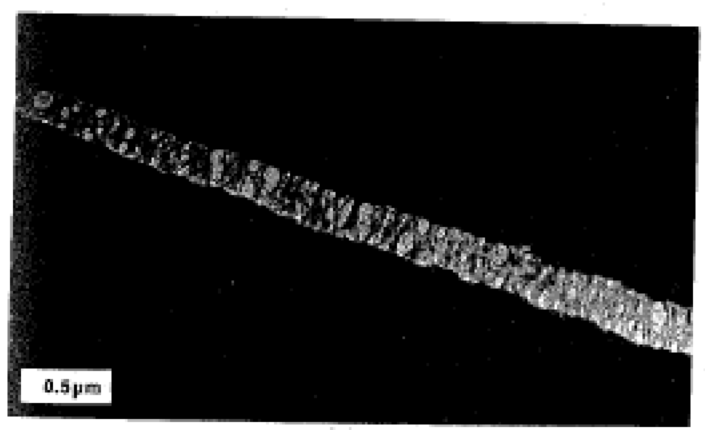



PS

Quinson, 2007




Craze evolution




Argon, 1977

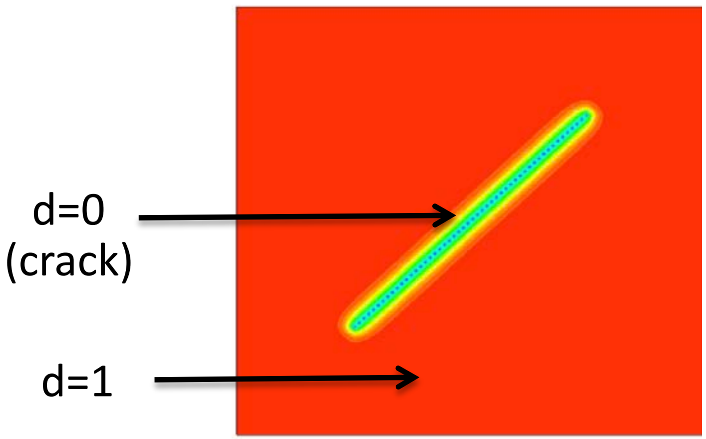
PS

# Phase field description of damage

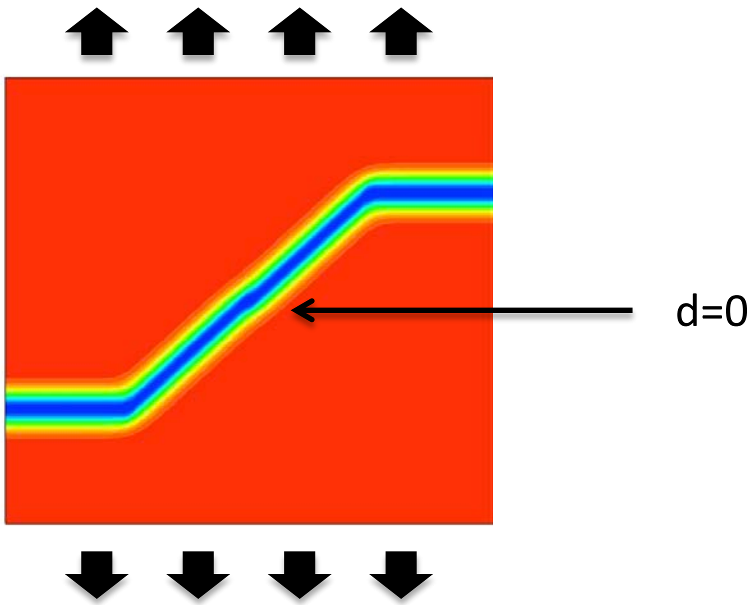
Griffith's theory $$W^{cr} = \int_{\Gamma} G_{cr}\, dx = \int_{V} G_{cr} \phi(d)\, dx$$

With a damage phase field $$\phi(d) = \frac{d^2}{2l_0} + \frac{l_0}{2}\left|\nabla d\right|^2$$

G. A. Fracfort and J. J. Marigo, 1998
M. J. Borden et al, 2012




Initial damage




Damage propagation

$$\sigma_{ij} = g(d)\left(\kappa\, \varepsilon^{v} \delta_{ij} + 2\mu\, \varepsilon^{d}_{ij}\right)$$

# Phase field description of damage

Solve structural problem coupled to an equation for the damage, d

$$\sigma_{ij} = \kappa\left(\varepsilon^{v} - \left\langle \varepsilon^{v} \right\rangle\right)\delta_{ij} + (1-d)^{2}\left(\underbrace{\kappa\left\langle \varepsilon^{v} \right\rangle\delta_{ij}}_{\text{}} + \underbrace{2\mu\varepsilon_{ij}^{d}}_{\text{}}\right)$$

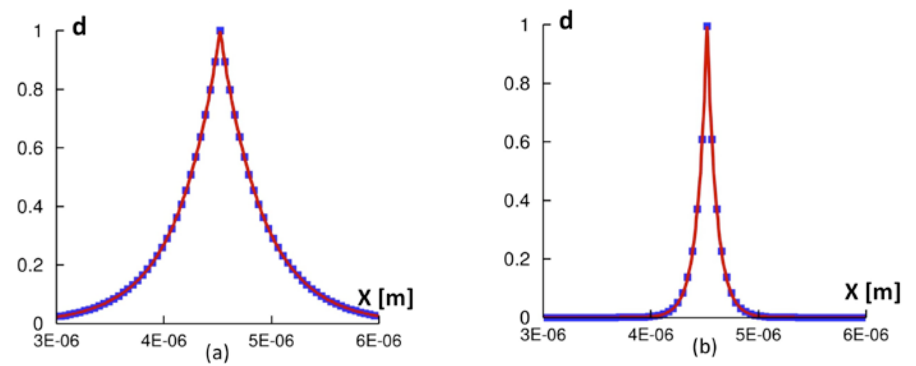
Loss of stiffness in tension only

Loss of stiffness in shear

With $\langle x \rangle = \begin{cases} x & if\ x > 0 \\ 0 & if\ x \le 0 \end{cases}$

$$\left(\frac{4l_0 a_0(\varepsilon)}{G} + 1\right)(1-d) - 4l_0^2 \frac{\partial^2 d}{\partial x_i \partial x_j} = 1$$

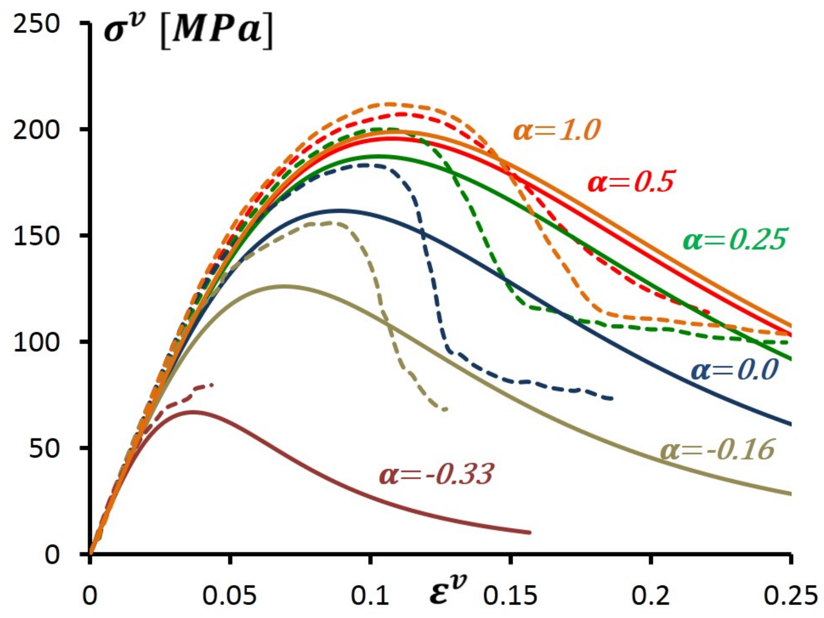
$$a_0(\varepsilon) = \frac{\kappa}{2}\left\langle \varepsilon^{v} \right\rangle^2 + \mu\varepsilon_{ij}^{d}\varepsilon_{ij}^{d}$$

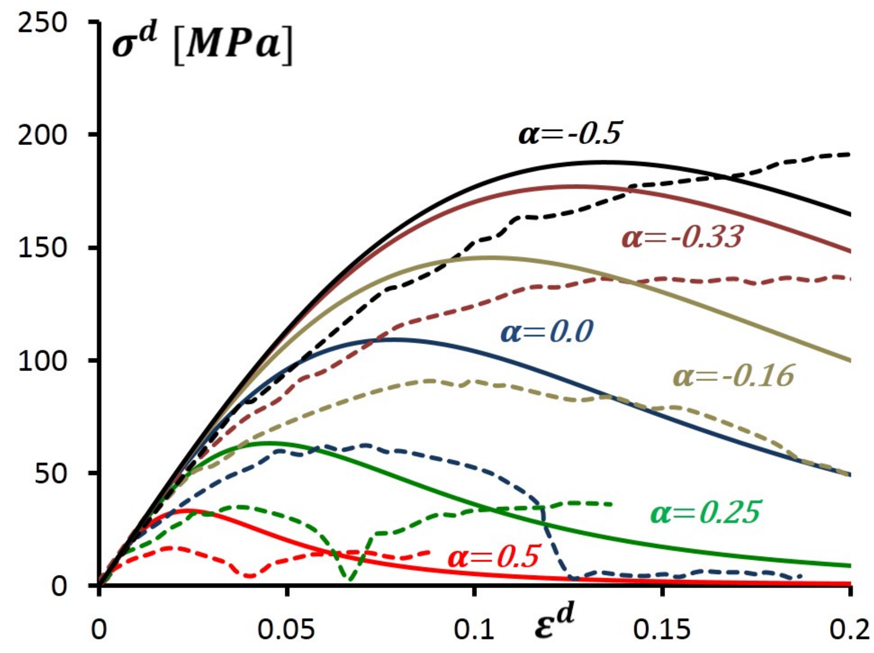



(a) ***$l_0$=200nm***, (b) ***$l_0$=45nm***

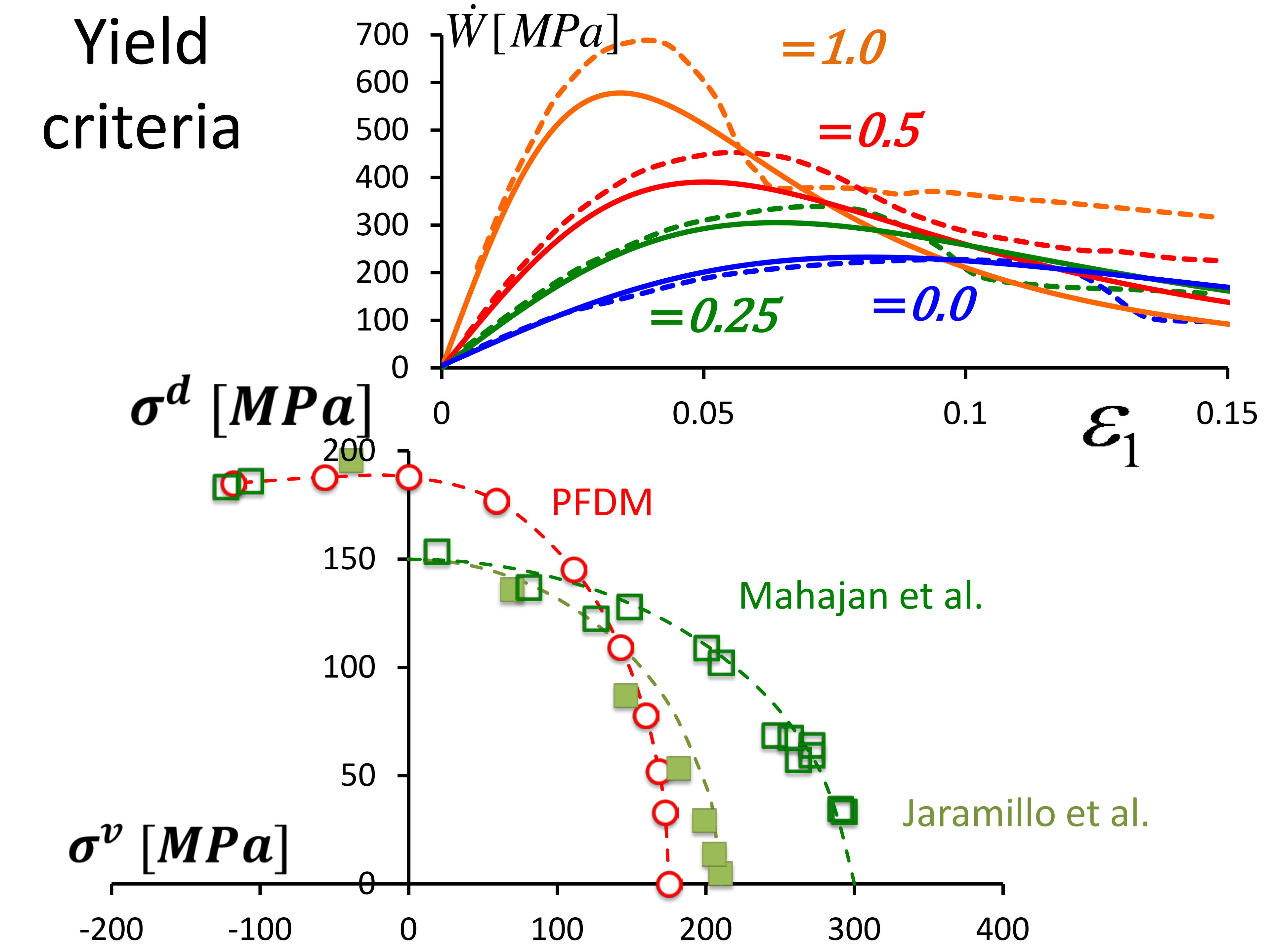
# Calibration with MD simulations

$$G_c/4l_0 = 45MPa$$



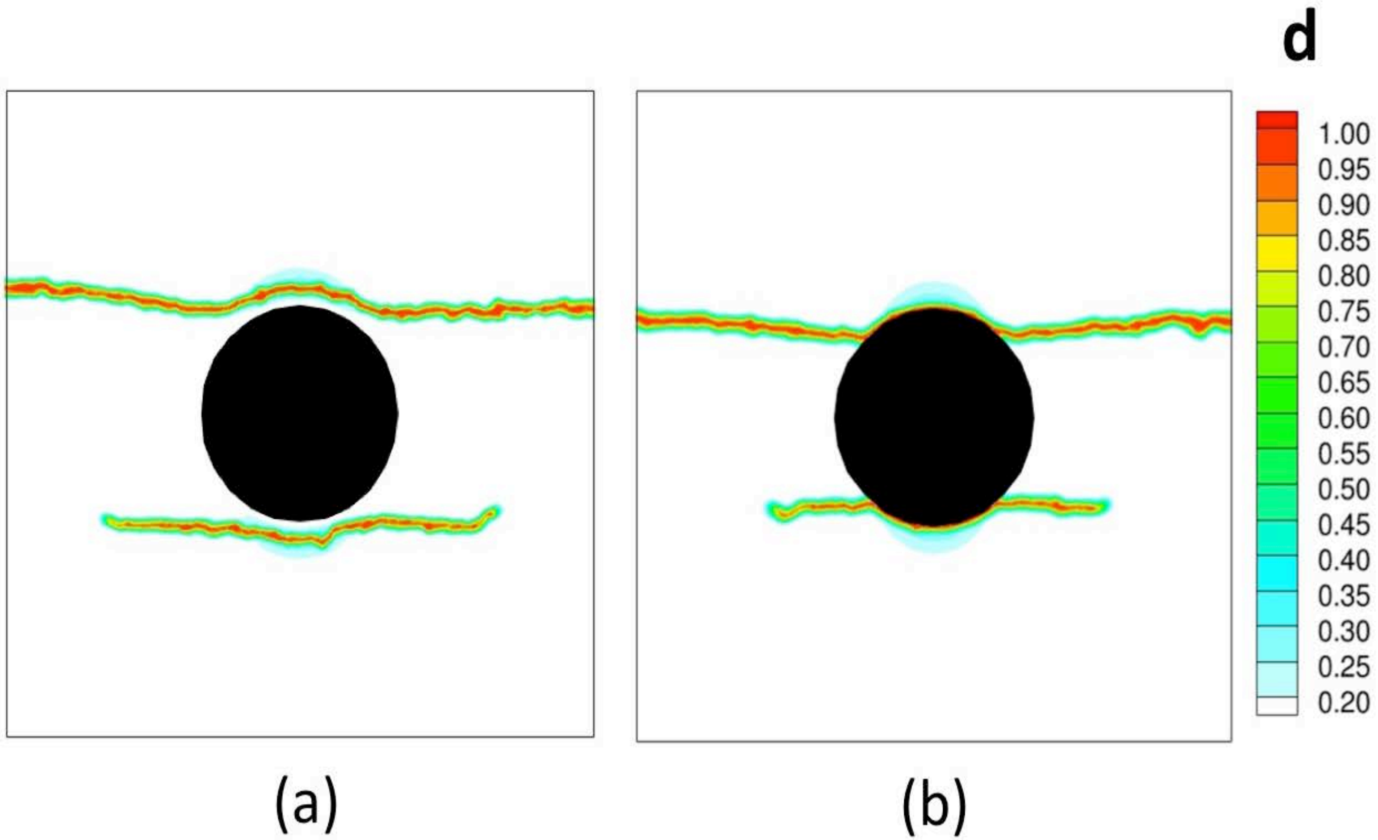




MD dashed lines (Jaramillo et al. 2012), Phase field solid lines (Xie et al, 2014)



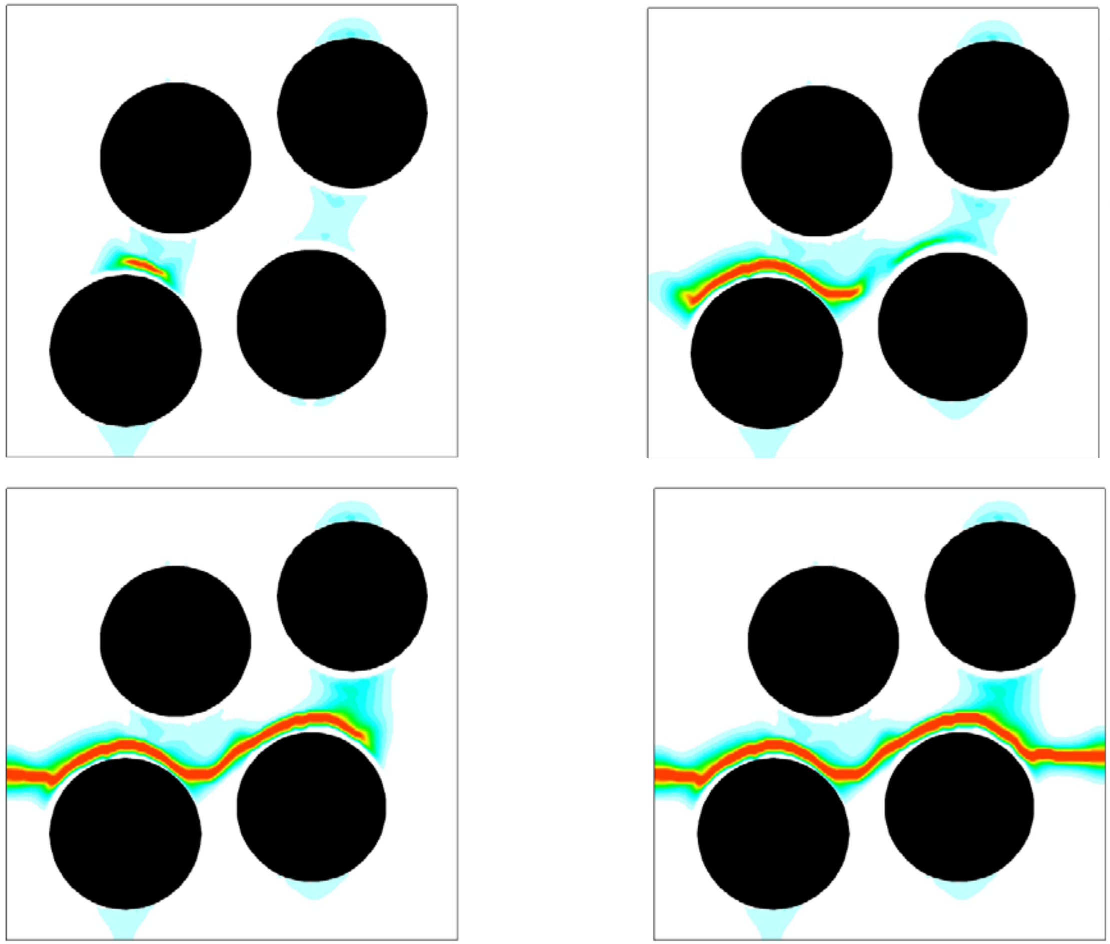
Yield criteria
$\dot{W}\,[MPa]$
700
600
500
400
300
200
100
0
=1.0
=0.5
=0.25
=0.0
0
0.05
0.1
0.15
$\varepsilon_1$
$\sigma^d\ [MPa]$
200
150
100
50
0
PFDM
Mahajan et al.
Jaramillo et al.
$\sigma^v\ [MPa]$
-200
-100
0
100
200
300
400

# Failure in composites

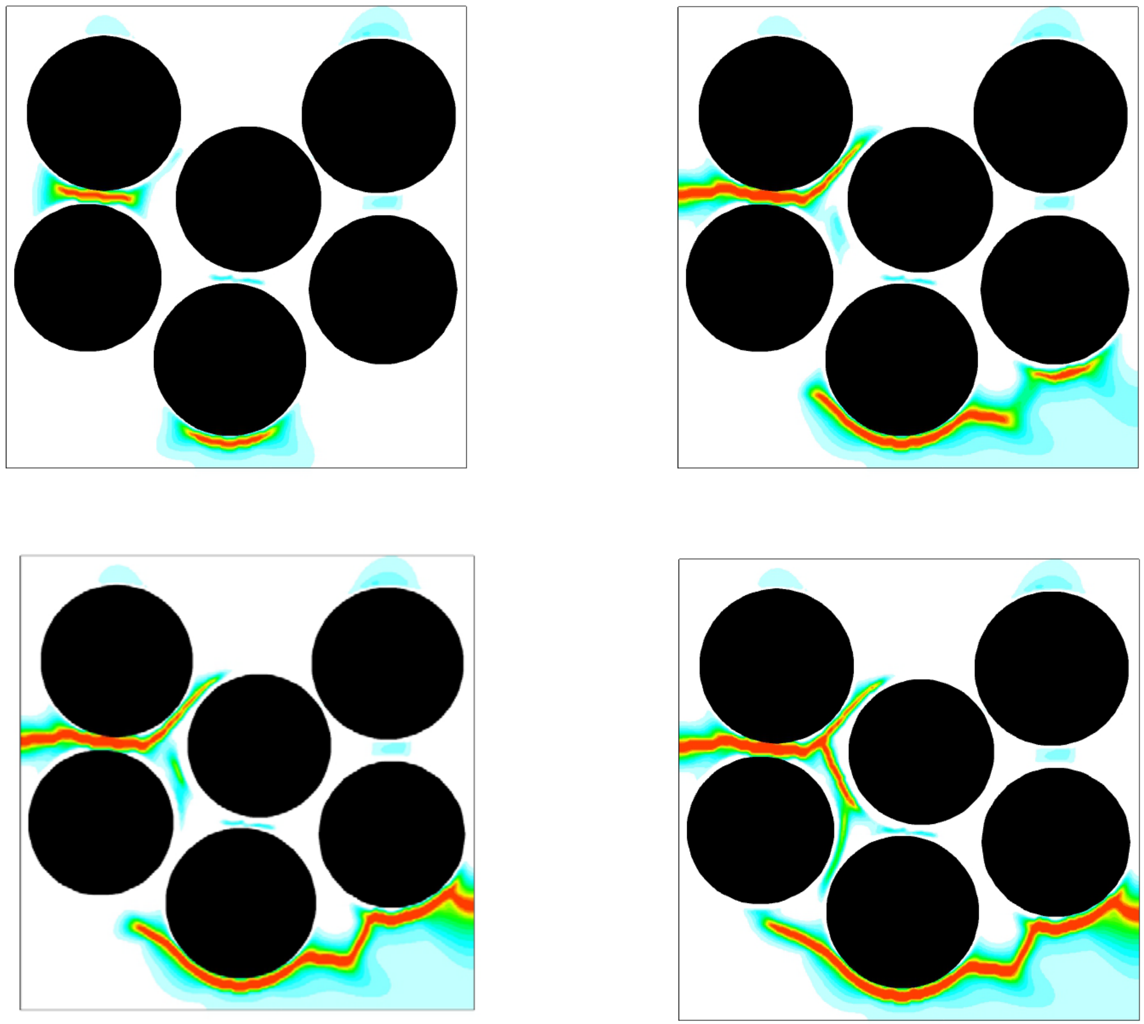



Predicted damage field for (a) perfectly bonded matrix/fiber interface and (b) damaged matrix/fiber interface.

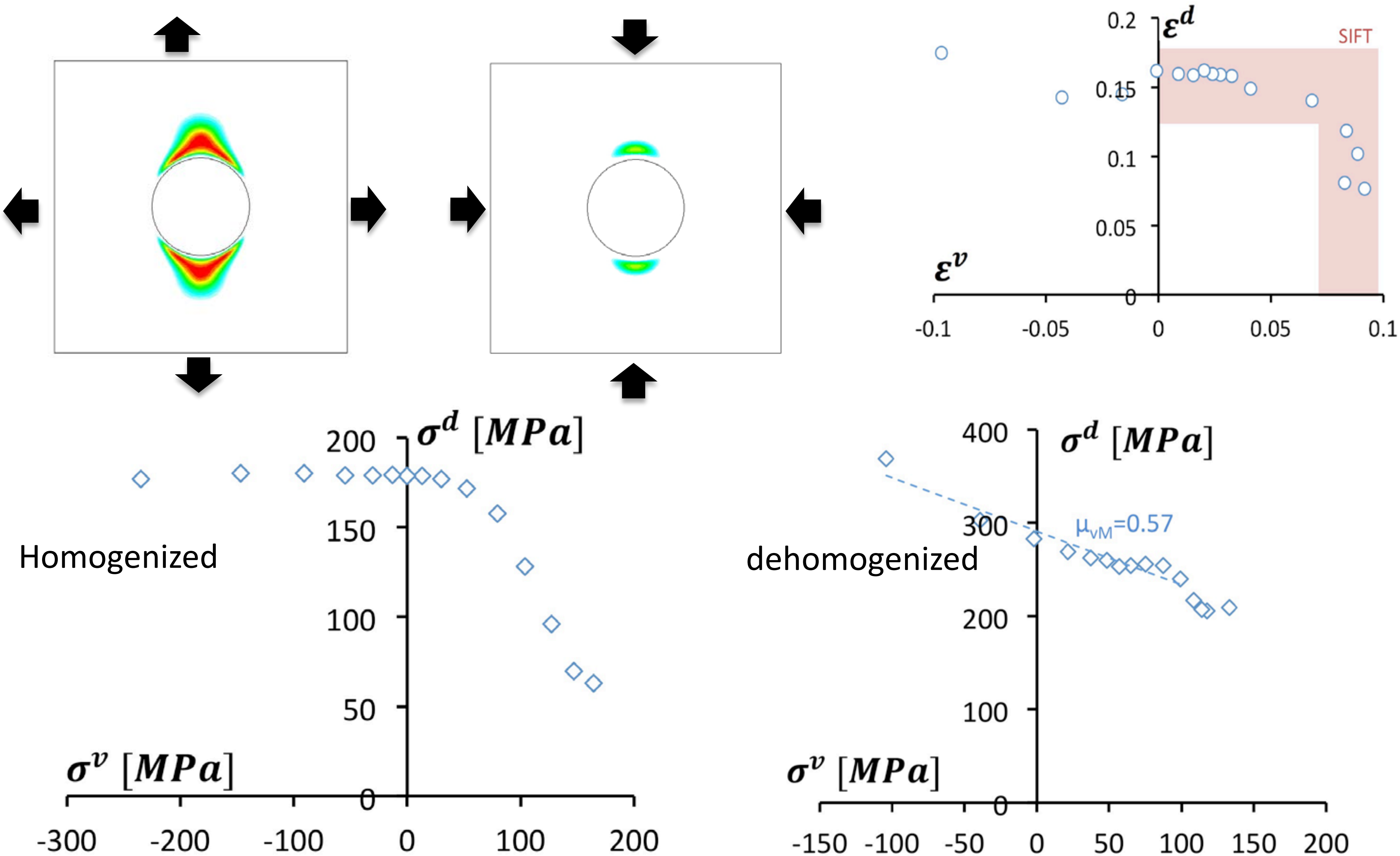
# Failure simulations in composites



# Failure simulations in composites



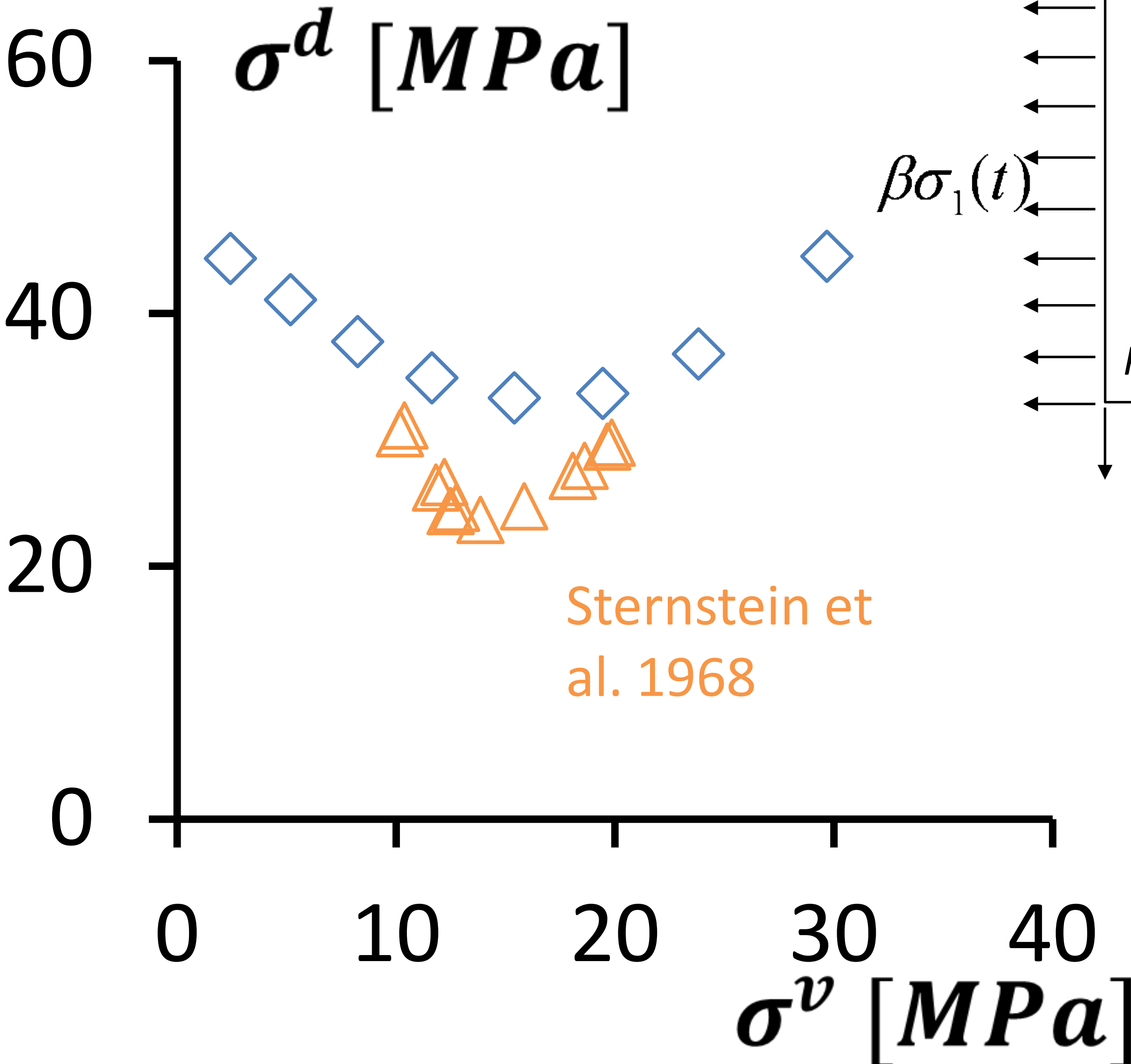
# Yield criteria in composite materials

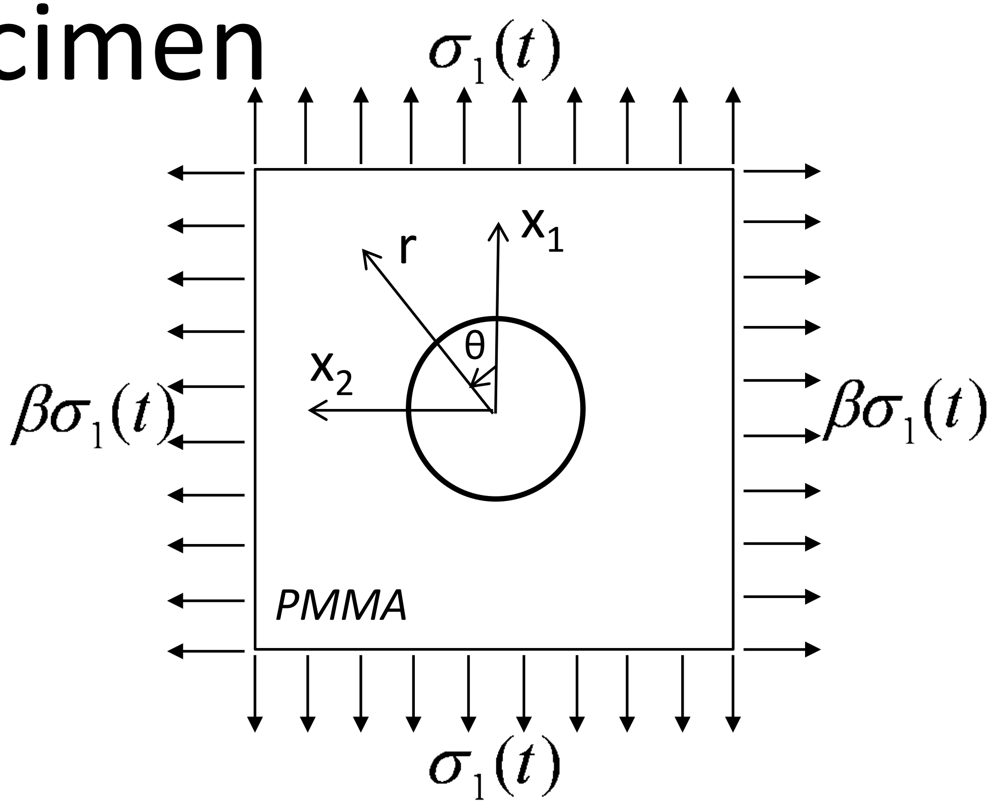


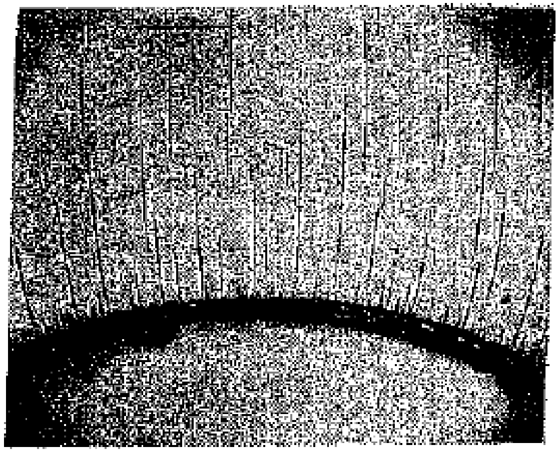

(a)

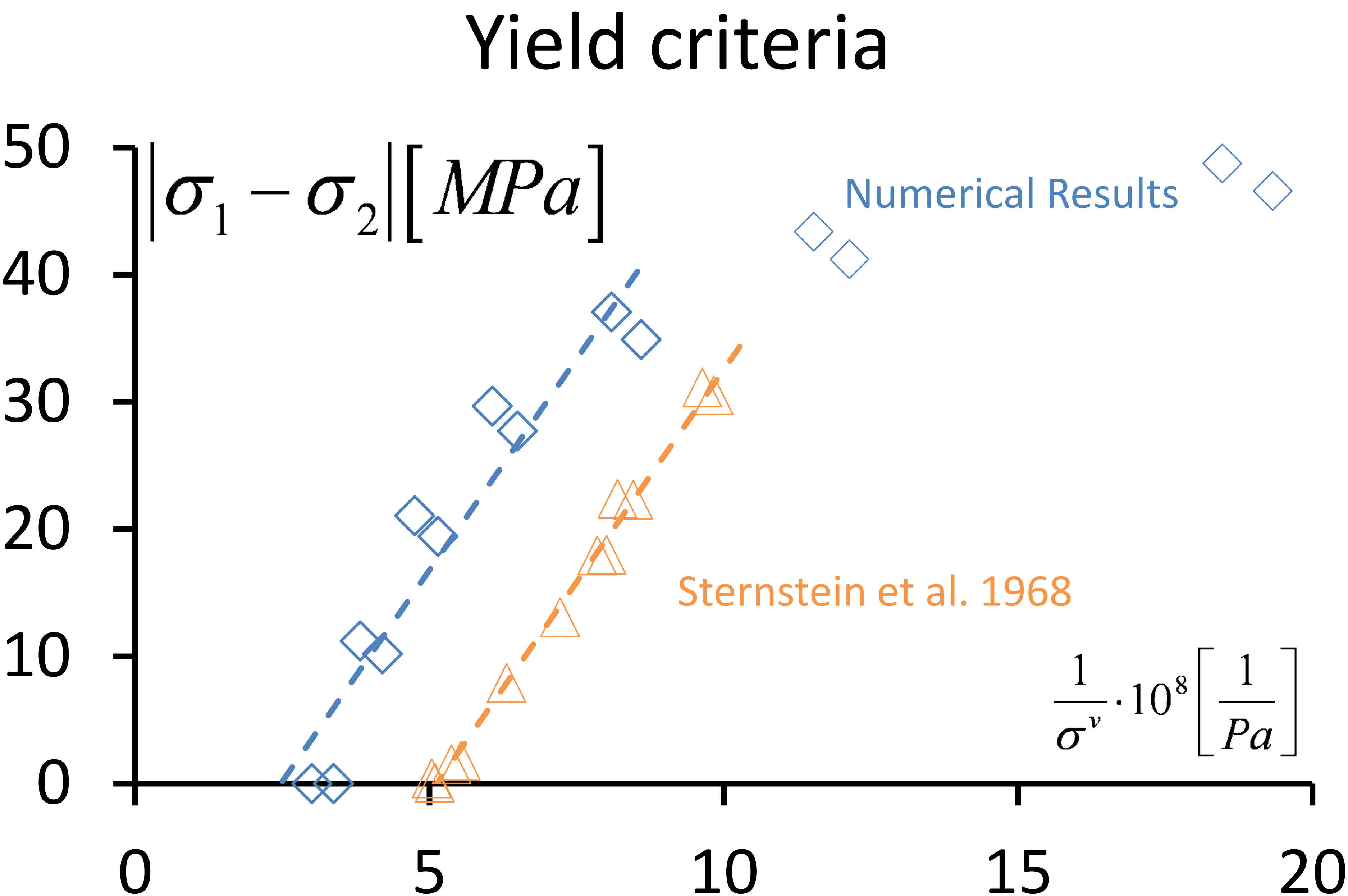
(b)

# Crazing in hole specimen





Yield criteria
50
40
30
20
10
0
0
5
10
15
20
$|\sigma_1 - \sigma_2| [MPa]$
Numerical Results
Sternstein et al. 1968
$\frac{1}{\sigma^v} \cdot 10^8 \left[\frac{1}{Pa}\right]$

# Yield condition