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"Jamming, Deformation and the Fracture in Amorphous Materials"

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Please note: These are preliminary notes intended for internal distribution only.

JAMMING, DEFORMATION, AND FRACTURE IN AMORPHOUS MATERIALS

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REFERENCES

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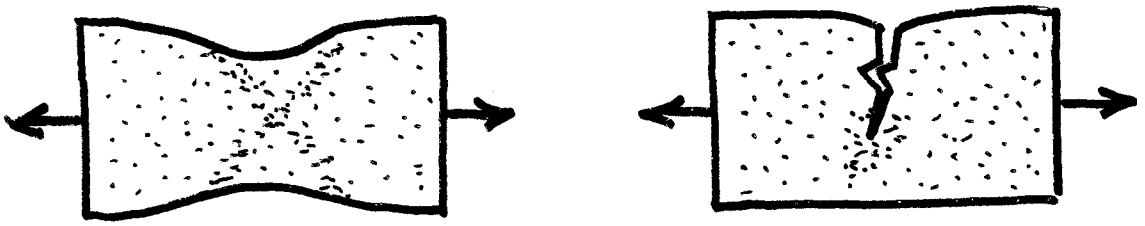
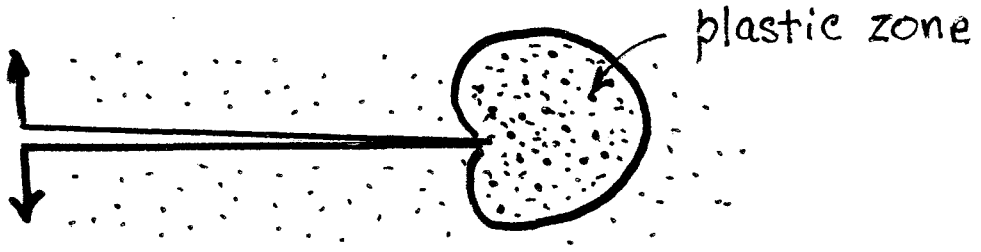
FUNDAMENTAL PUZZLES IN FRACTURE DYNAMICS

How can we understand brittle and ductile behaviors, especially in noncrystalline solids?



What is the origin of dynamic instabilities in brittle fracture?

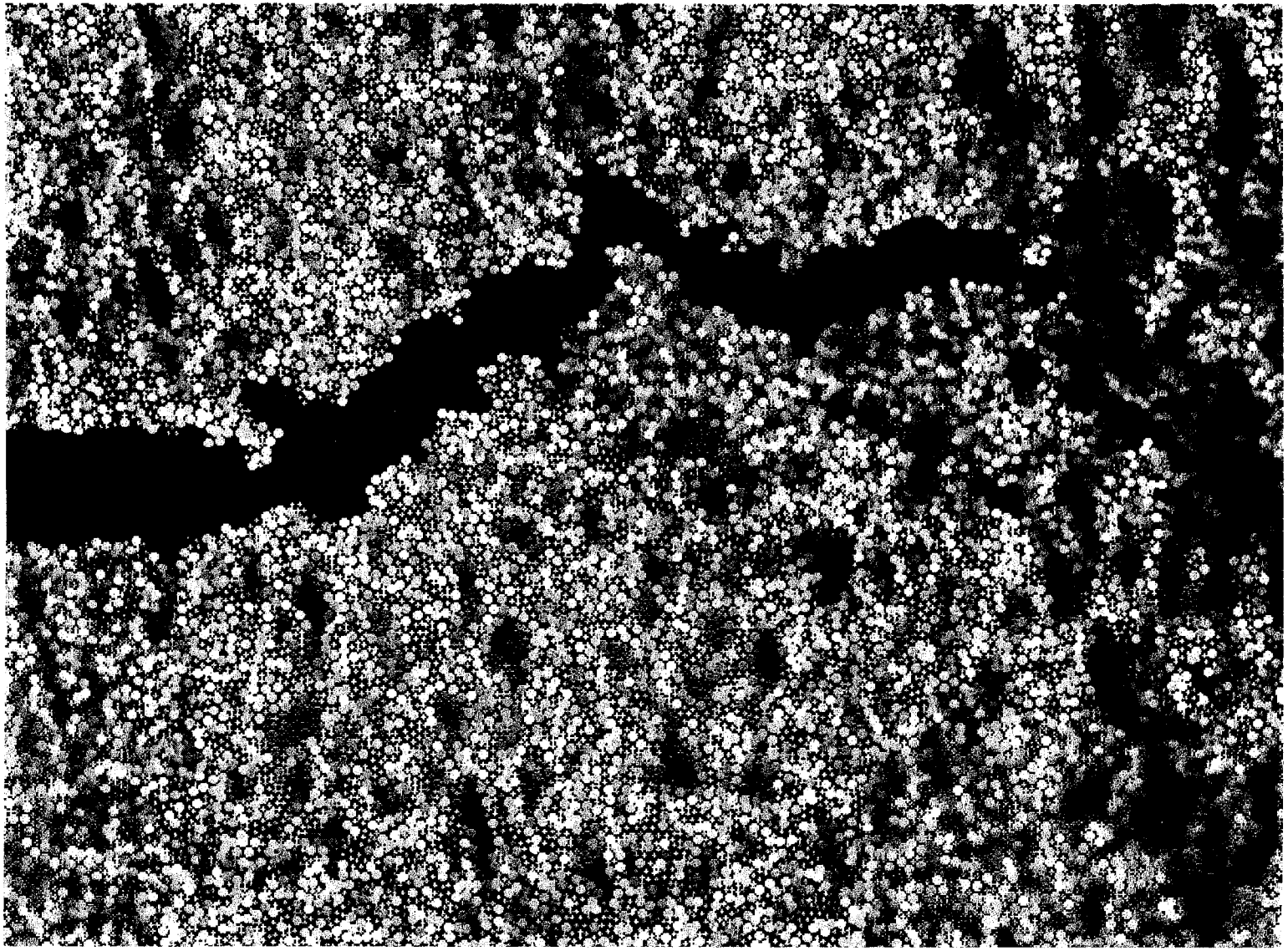
If there is always a plastic yield stress, how can a (higher)? breaking stress be transmitted to a crack tip?



Closeup of Crack Tip In Brittle Fracture

M. Falk

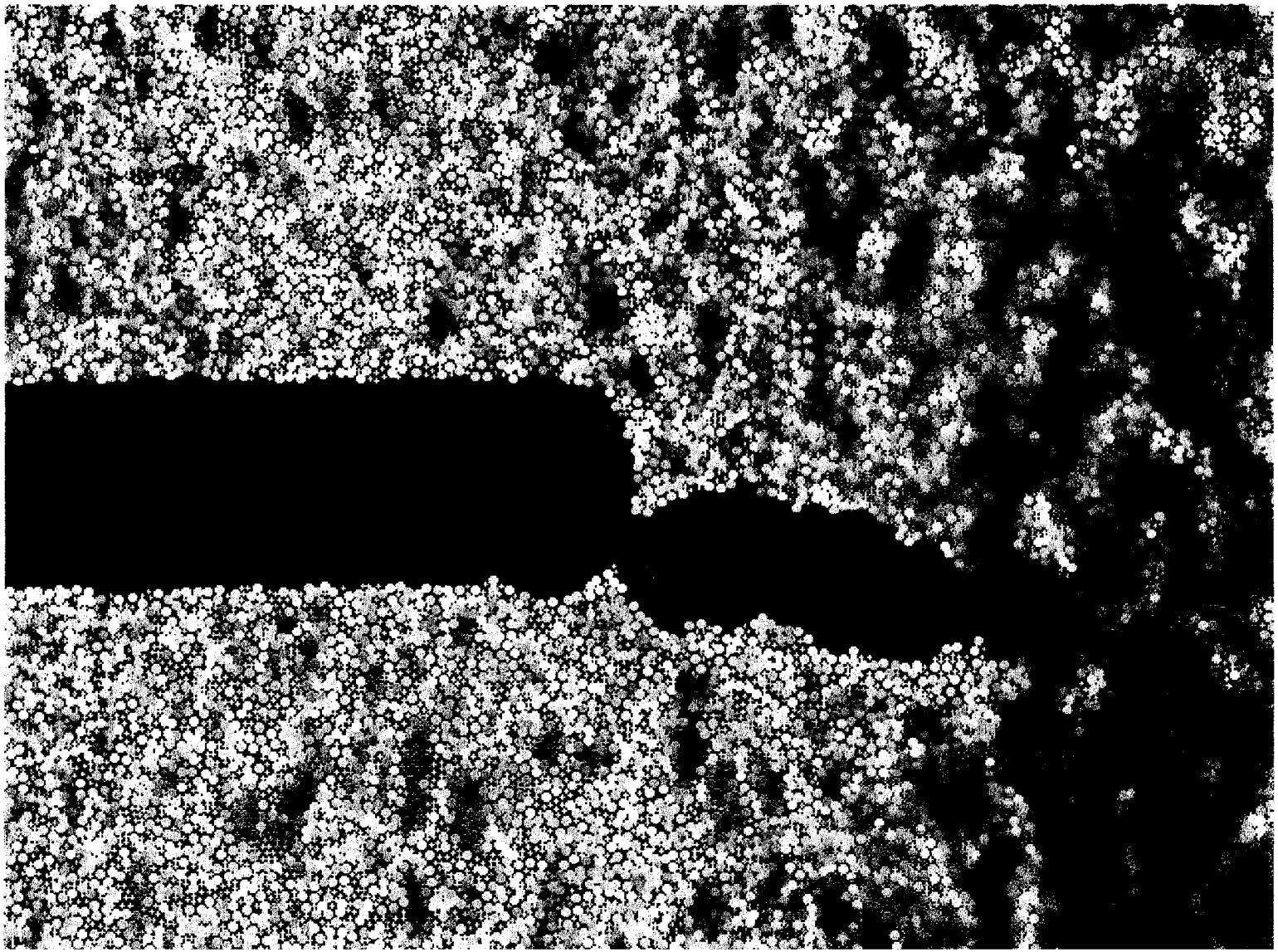
10^5 Molecule 2D Compressed LJ Solid with distribution of molecular radii colored by σ_{yy} – red = compression, blue = tension



Closeup of Crack Tip In Ductile Fracture

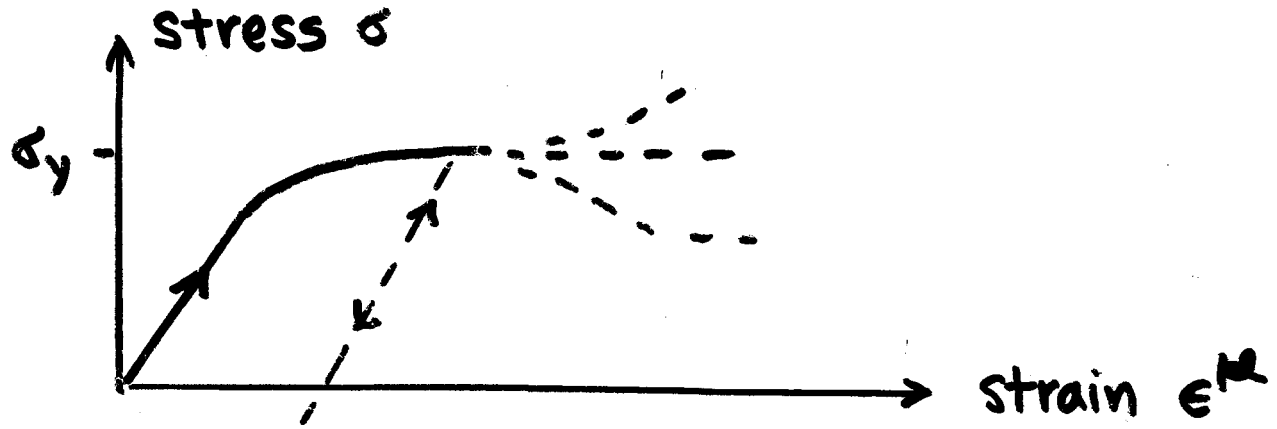
M.Falk

10^5 Molecule 2D LJ Solid with distribution of molecular radii colored by σ_{yy} – red = compression, blue = tension



CONVENTIONAL DESCRIPTIONS OF PLASTICITY

Time - Independent



Rate - Dependent

What would be a suitable form for a theory of plasticity?

Equations of motion:

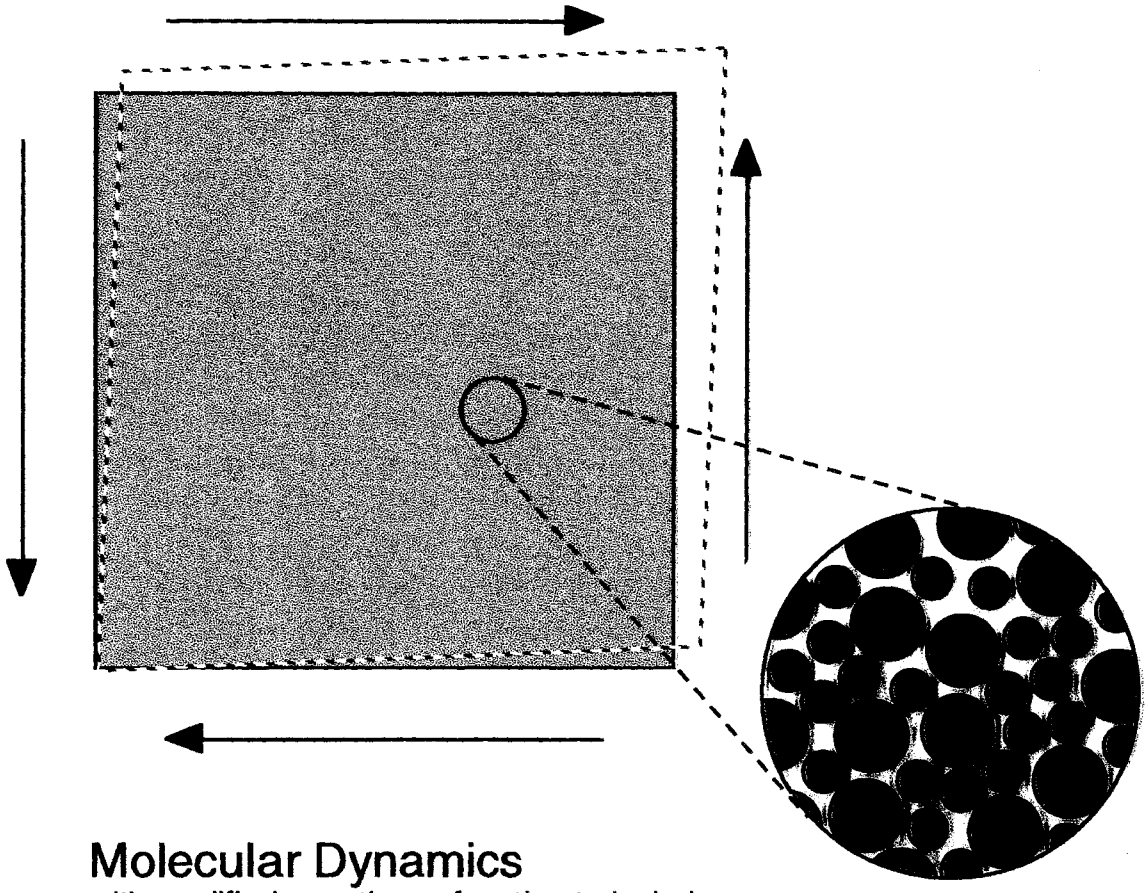
$$\frac{d\epsilon^{pl}}{dt} = F(\sigma, \Delta, \dots)$$

$$\frac{d\Delta}{dt} = G(\sigma, \Delta, \dots)$$

σ = stress , ϵ^{pl} = plastic strain

$\Delta, \dots$ = internal state variables (not including ϵ^{pl})

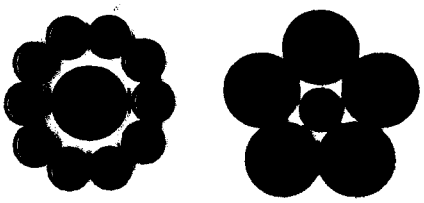
2-D 2-Component LJ Solid Under Applied Simple Shear



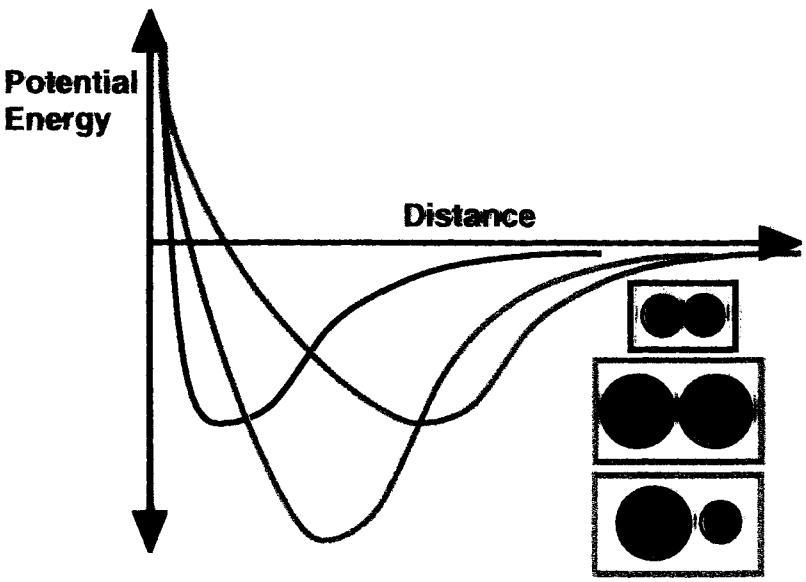
Molecular Dynamics

with modified equations of motion to include:

- Thermostat
- Pressure-Stress Barostat

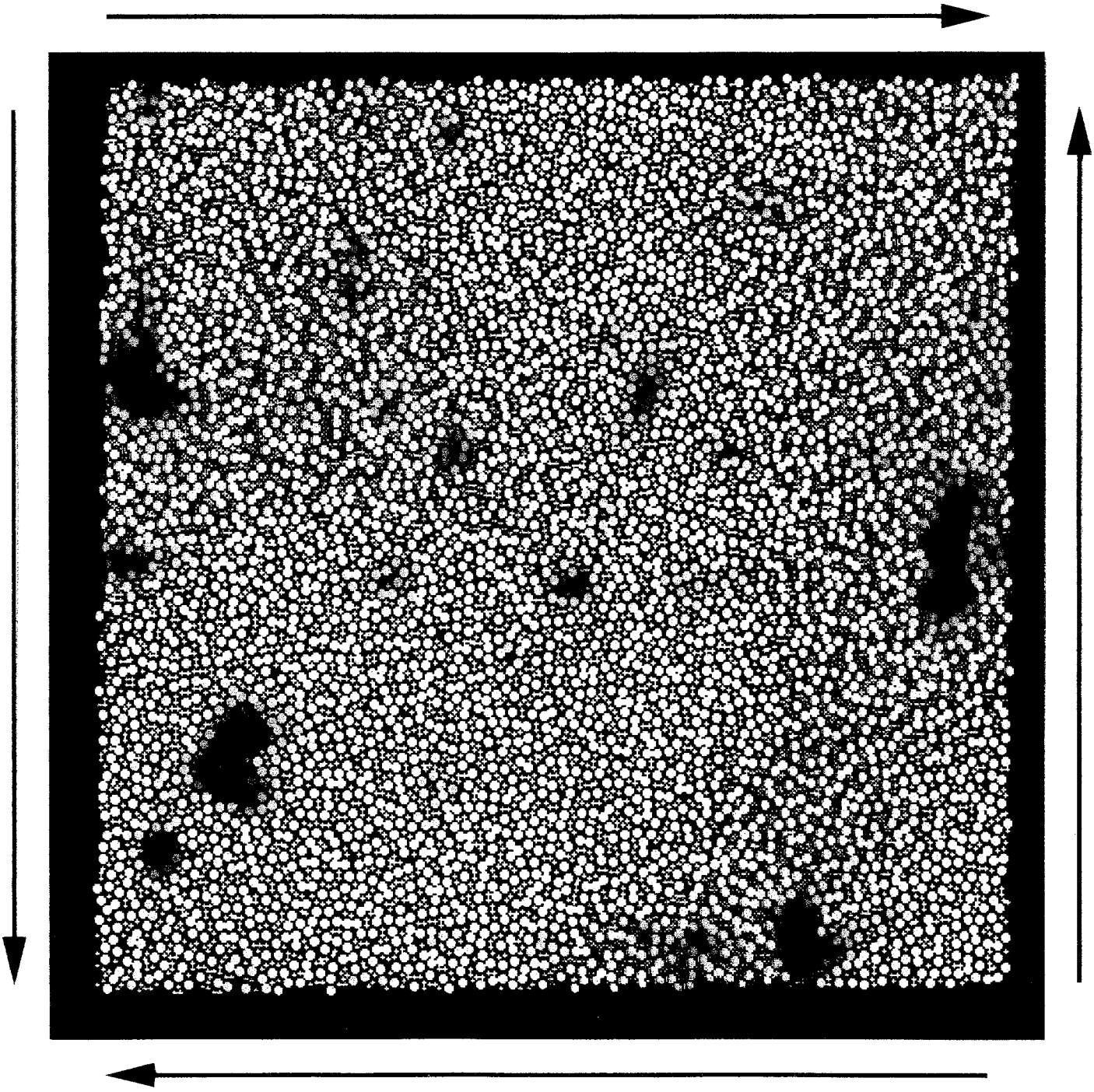


Quasicrystalline Ground State



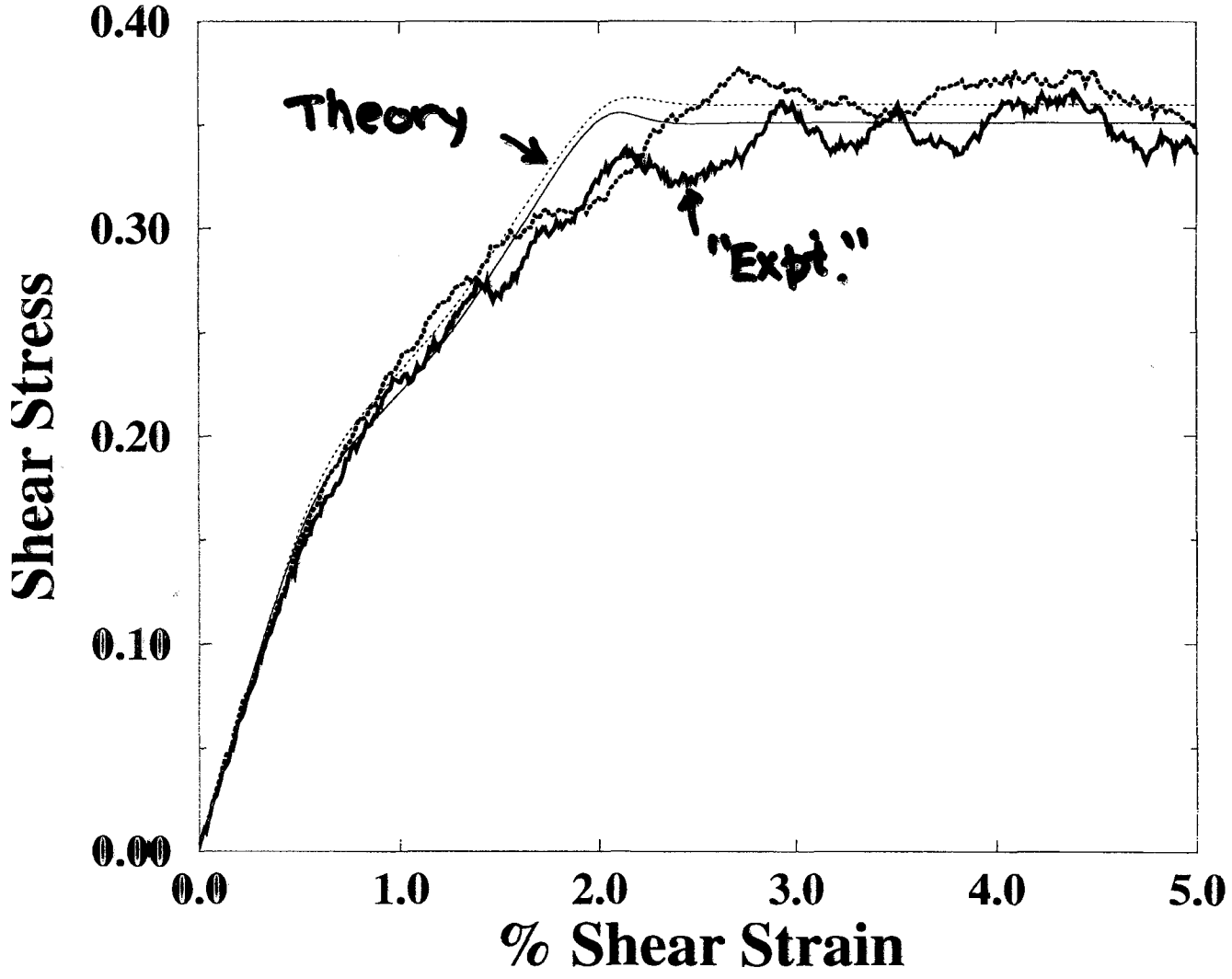
Periodic Cell Under Applied Pure Shear Stress

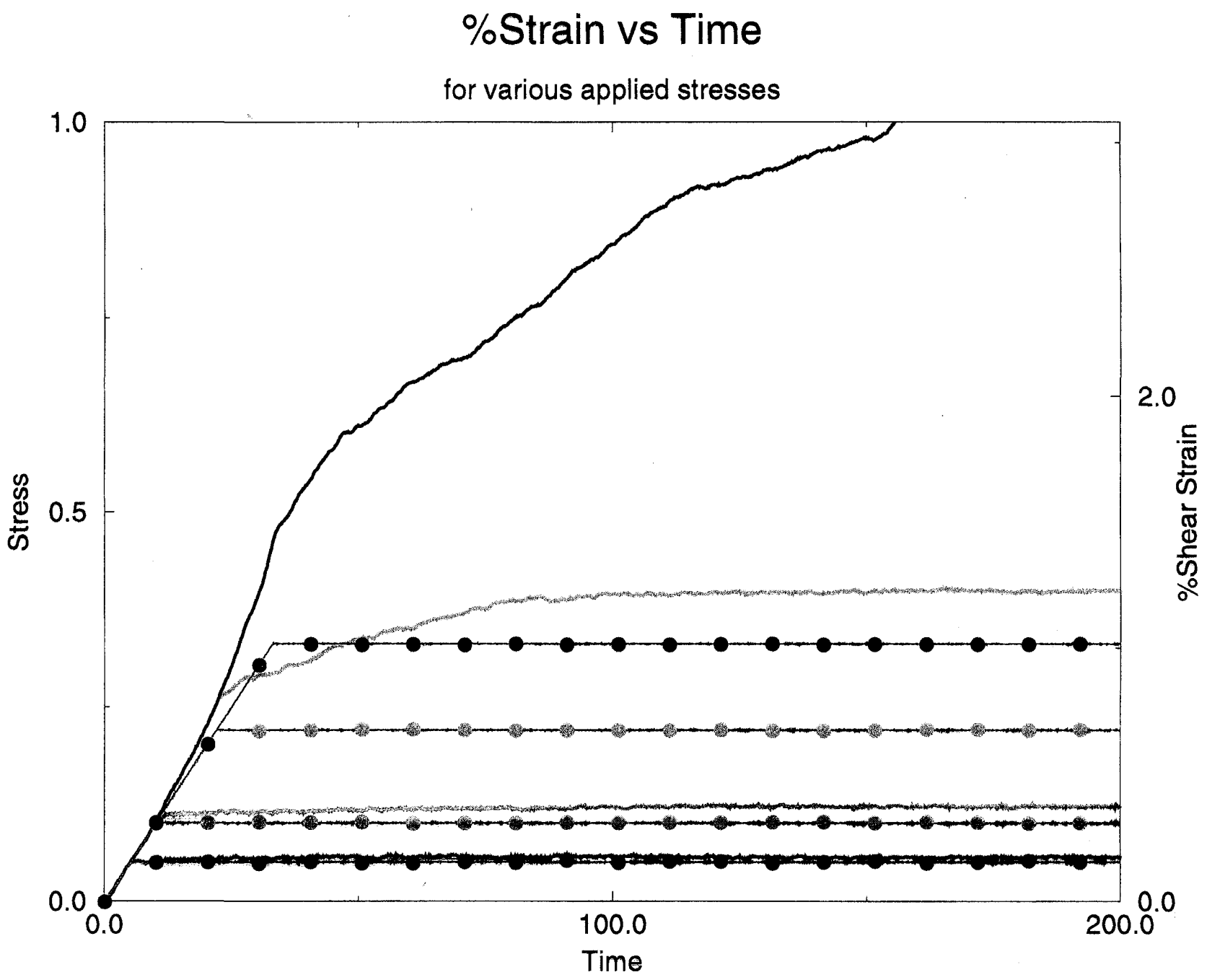
red regions denote areas of local deviation from affine deformation

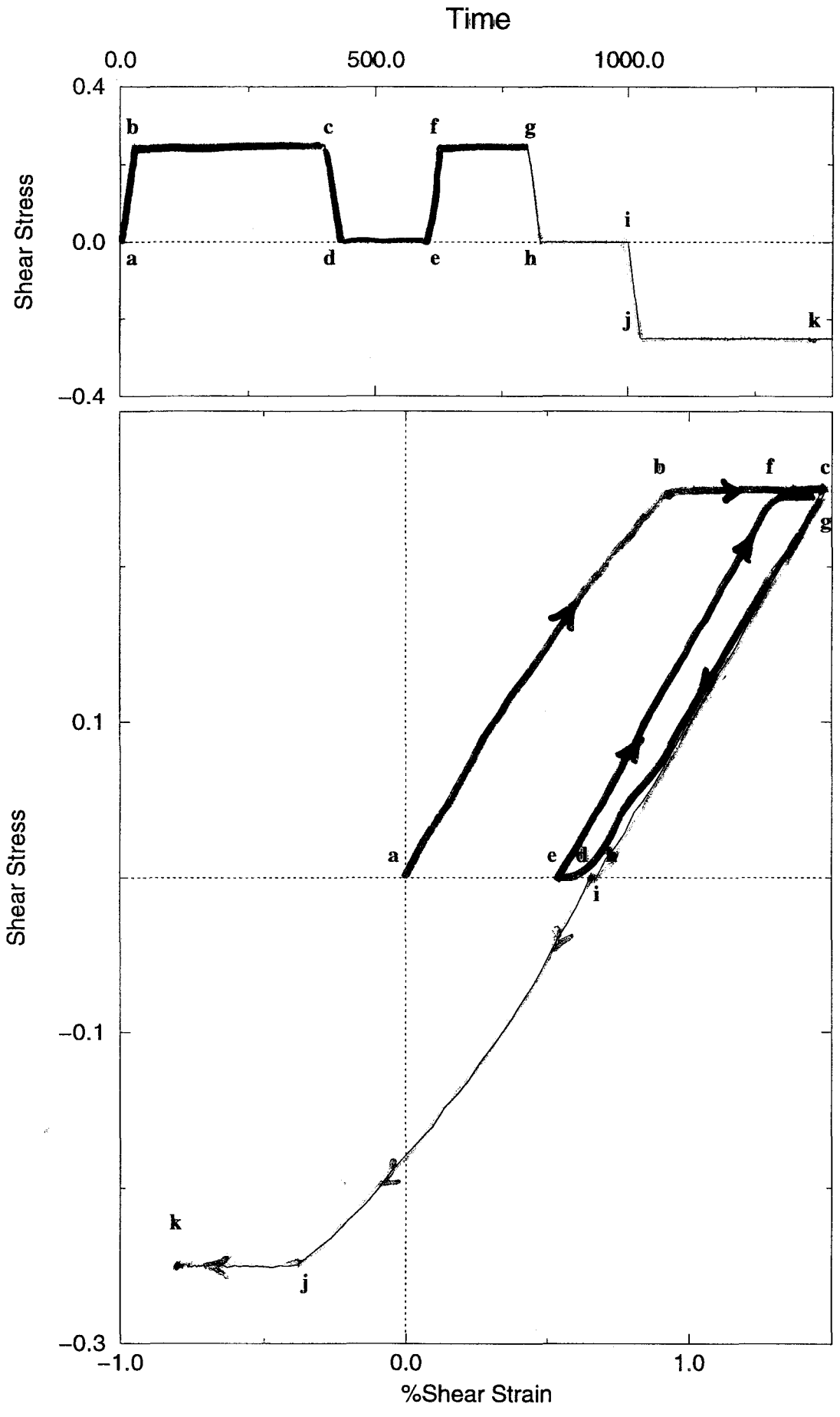


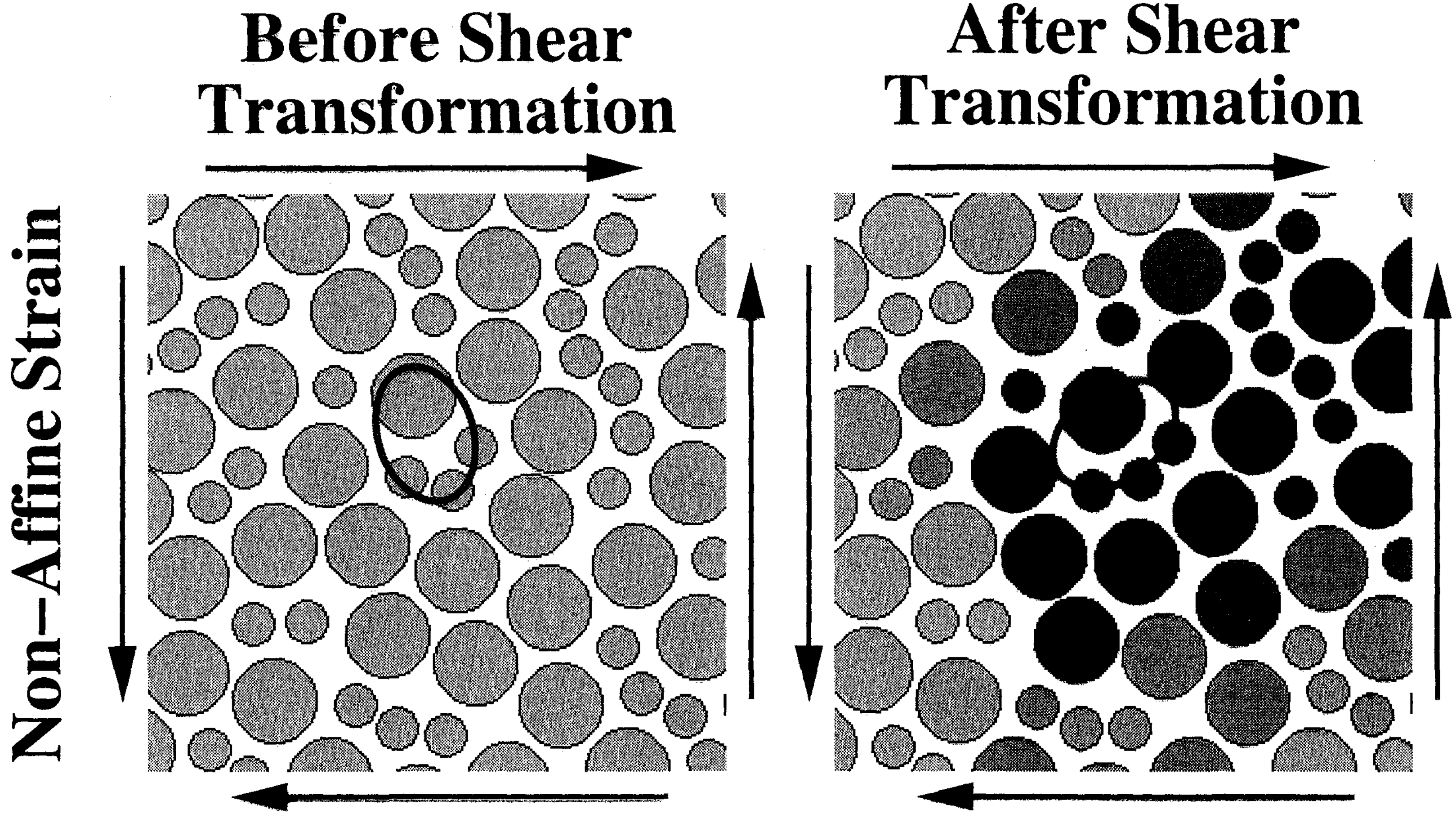
STRESS-STRAIN CURVES FOR TWO DIFFERENT STRAIN RATES

$\dot{\varepsilon} = 10^{-4}, 2\times10^{-4}$ in dimensionless (atomic scale) units

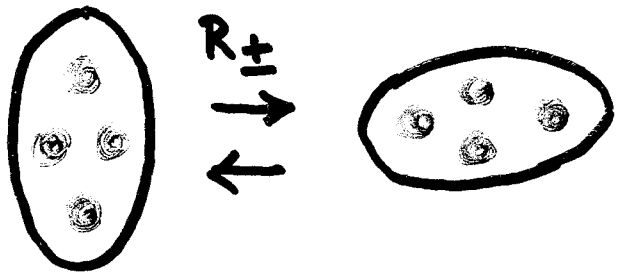



%Strain vs Time
for various applied stresses
1.0
0.5
0.0
Stress
0.0
100.0
200.0
Time
2.0
0.0
%Shear Strain


Time
0.0
500.0
1000.0
0.4
0.0
−0.4
Shear Stress
a
b
c
d
e
f
g
h
i
j
k
0.1
−0.1
−0.3
−1.0
0.0
1.0
%Shear Strain


Before Shear Transformation
After Shear Transformation
Non–Affine Strain

STZ SUMMARY



strain rate $\dot{\varepsilon}^{pl} \sim R_+ n_+ - R_- n_-$

$$R_\pm(s) = R_0 \exp\left[-\Delta V^*(s)/\sigma_f\right]$$

$n_\pm$ = density of STZs , s = deviatoric stress

$$\dot{n}_\pm = R_\mp n_\mp - R_\pm n_\pm + (\dot{\varepsilon}^{pl} s)(A_{cr} - A_{ann} n_\pm)$$

↑ creation & annihilation rates ~ rate of plastic work

$$n_\infty \equiv \frac{2A_{cr}}{A_{ann}} \qquad \Delta \equiv \frac{n_- - n_+}{n_\infty} \qquad \Lambda \equiv \frac{n_+ + n_-}{n_\infty}$$

Quasilinear approximation : { Uniform system; No hysteresis

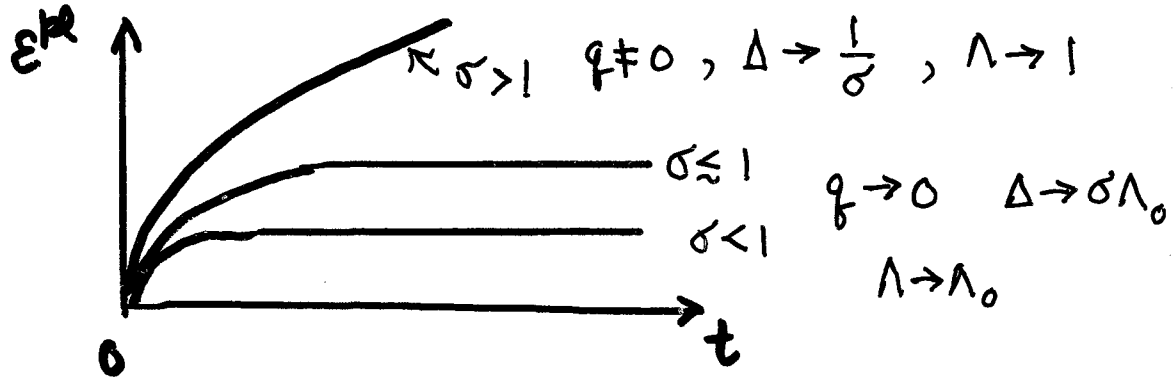
$$\dot{\varepsilon}^{pl} \sim \sigma\Lambda - \Delta \equiv q(\sigma, \Delta, \Lambda) \qquad \sigma \equiv \frac{s}{s_y}$$

$\dot{\Delta} = q(1 - \sigma\Delta)$ $\quad$ $\Delta \sim$ orientation of STZs

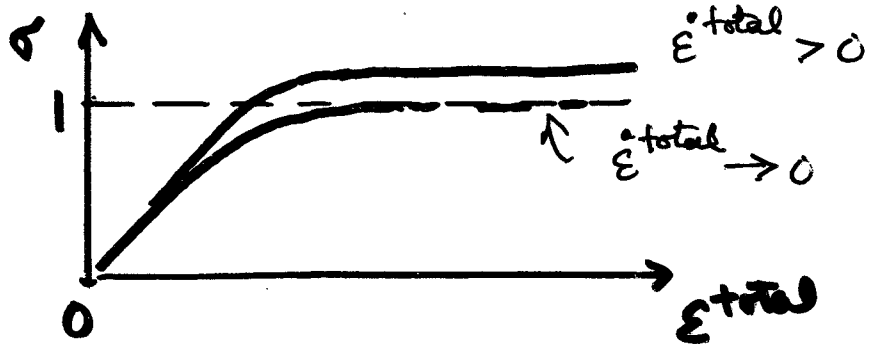
$\dot{\Lambda} = \sigma q(1 - \Lambda)$ $\quad$ $\Lambda \sim$ density of STZs

SPATIALLY UNIFORM STZ MODEL

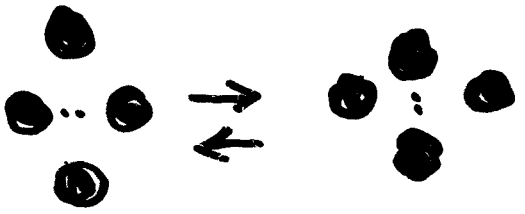
Constant stress (creep tests)



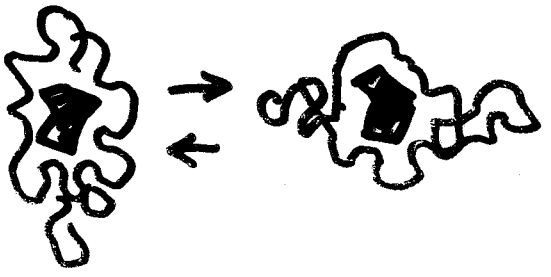
Strain rate $\dot{\varepsilon}^{total}$ = constant



Memory effects come from a nonlinear rate factor that governs switching from one state to another in "two-state" systems.



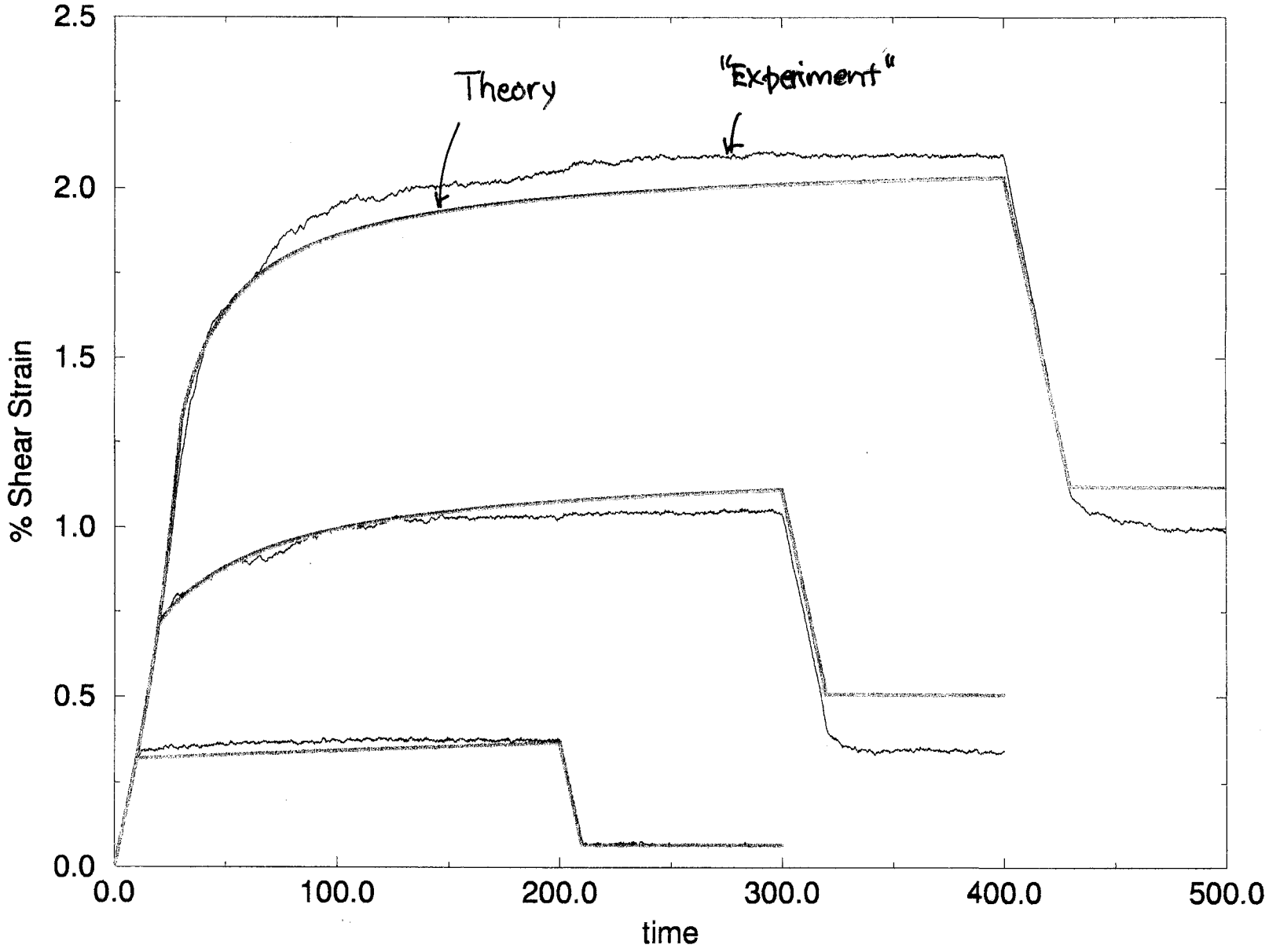
STZ Model

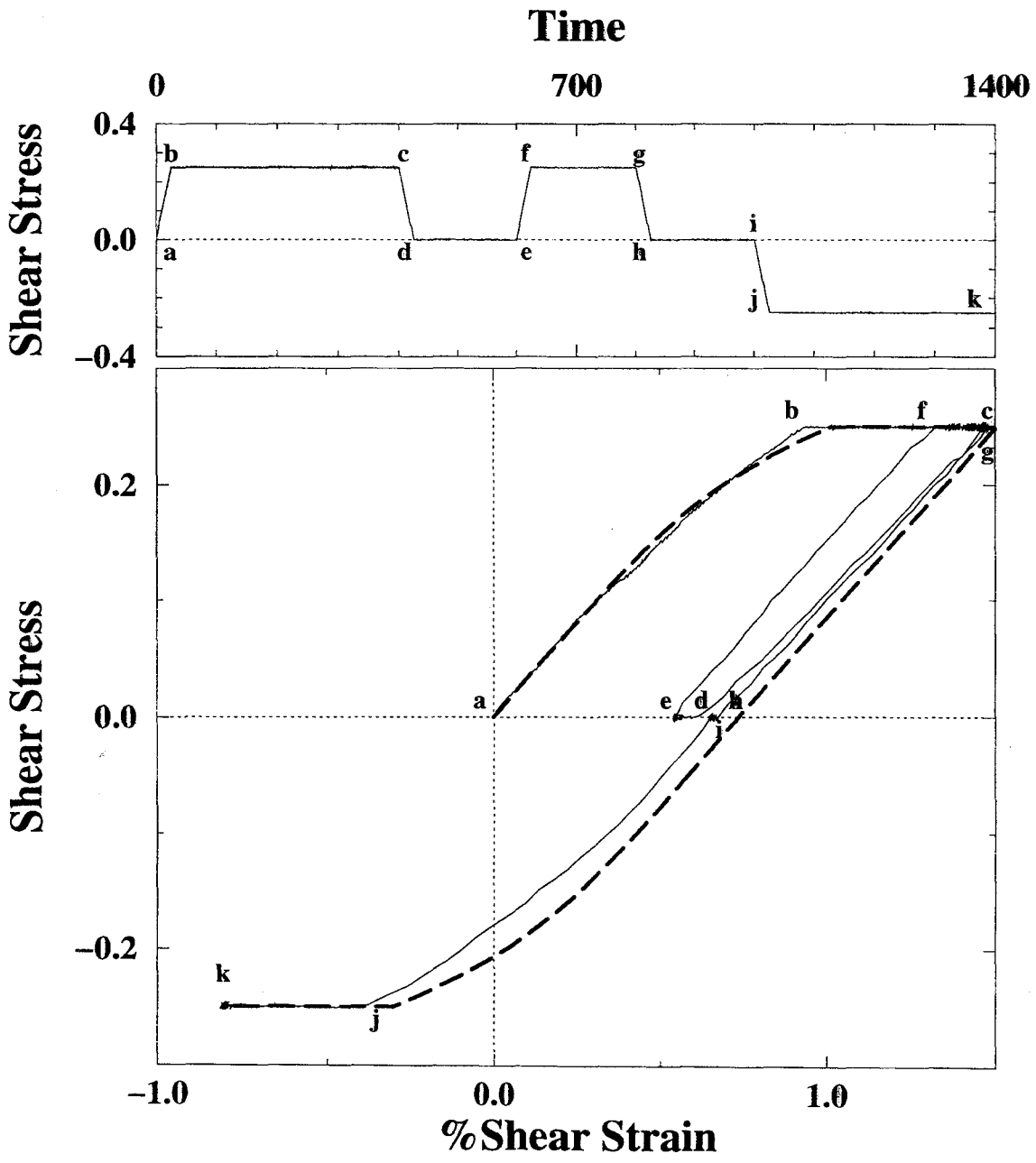


Dislocations near defects

Activation mechanism (free volume version)

$$R_{\pm} \sim e^{-\Delta V^{*}(\pm s)/v_f}$$


Theory
"Experiment"
% Shear Strain
time
0.0
0.5
1.0
1.5
2.0
2.5
0.0
100.0
200.0
300.0
400.0
500.0


Time
0
700
1400
Shear Stress
0.4
0.0
−0.4
a
b
c
d
e
f
g
h
i
j
k
Shear Stress
0.2
0.0
−0.2
−1.0
0.0
1.0
%Shear Strain

RESULTS

- Two-state systems imply "jamming" at low, fixed stress.

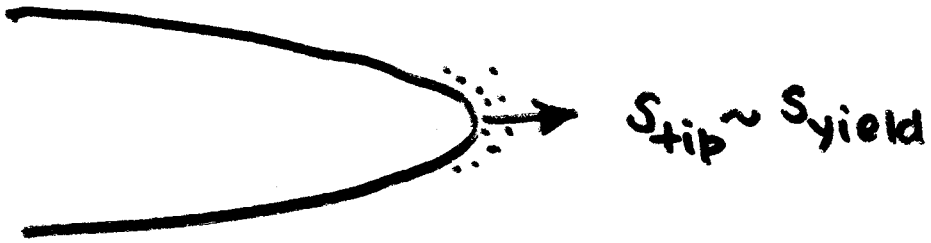
- Annihilation and creation terms imply that there is a yield stress above which the plastic strain rate is nonzero for fixed stress.

- Strong state dependence of the transition rates R(±) produces memory effects.

THE TIP-STRESS PUZZLE

(NEW CONJECTURES)

Crack advance may be governed primarily by (something like?) plastic deformation of the material near the crack tip.

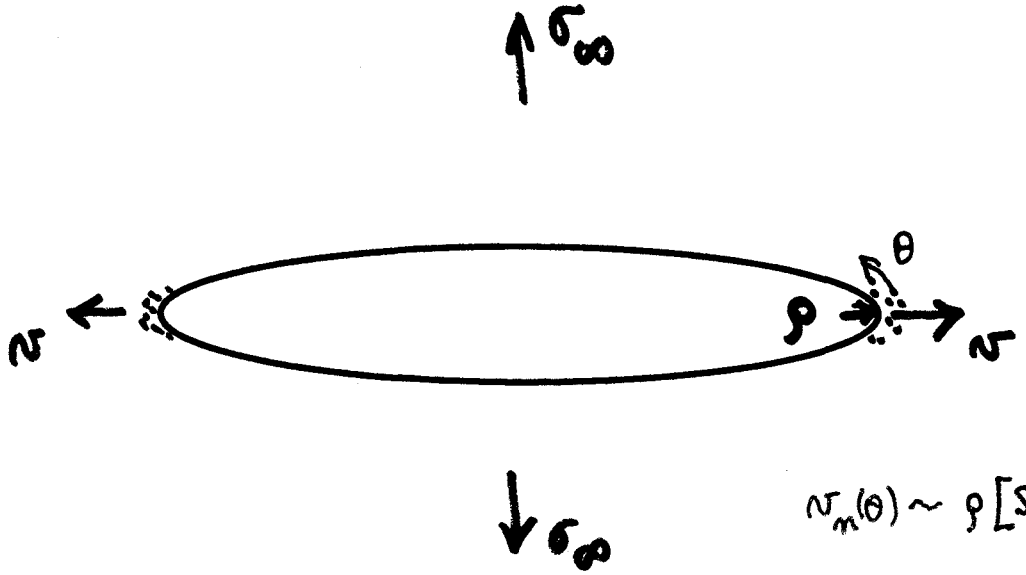


A nonzero radius of curvature of the crack tip is an essential dynamical variable. It regularizes stress singularities. It controls the plastic deformation rate, and therefore controls the crack speed.

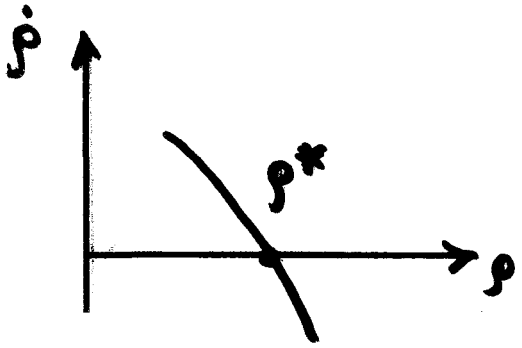
Viscoplasticity and the Dynamics of Brittle Fracture

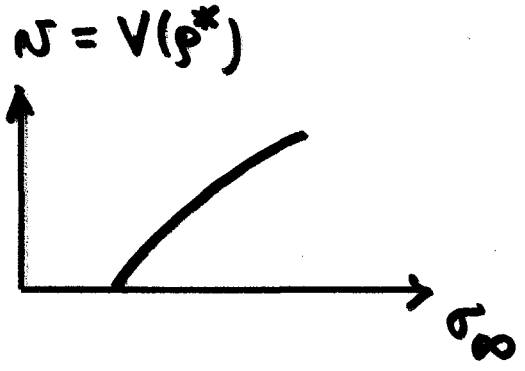
J.S.L.

Long, thin elliptical hole :



$$\sigma_m(\theta) \sim \rho\,[S_{\theta\theta}(\theta) - S_y]$$





Stable fixed point at finite ρ for $S_y \neq 0$.