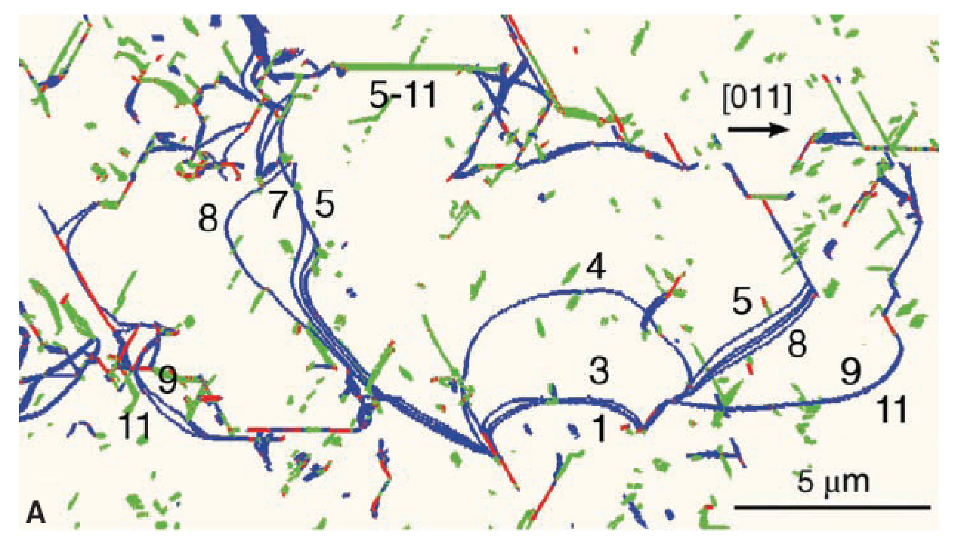
Nonequilibrium Thermodynamics of Dislocation-Mediated Plasticity



J.S. Langer

KITP 10/17/2014

Thermodynamic theory of dislocation-mediated plasticity, Acta Materialia 58, 3718 (2010)

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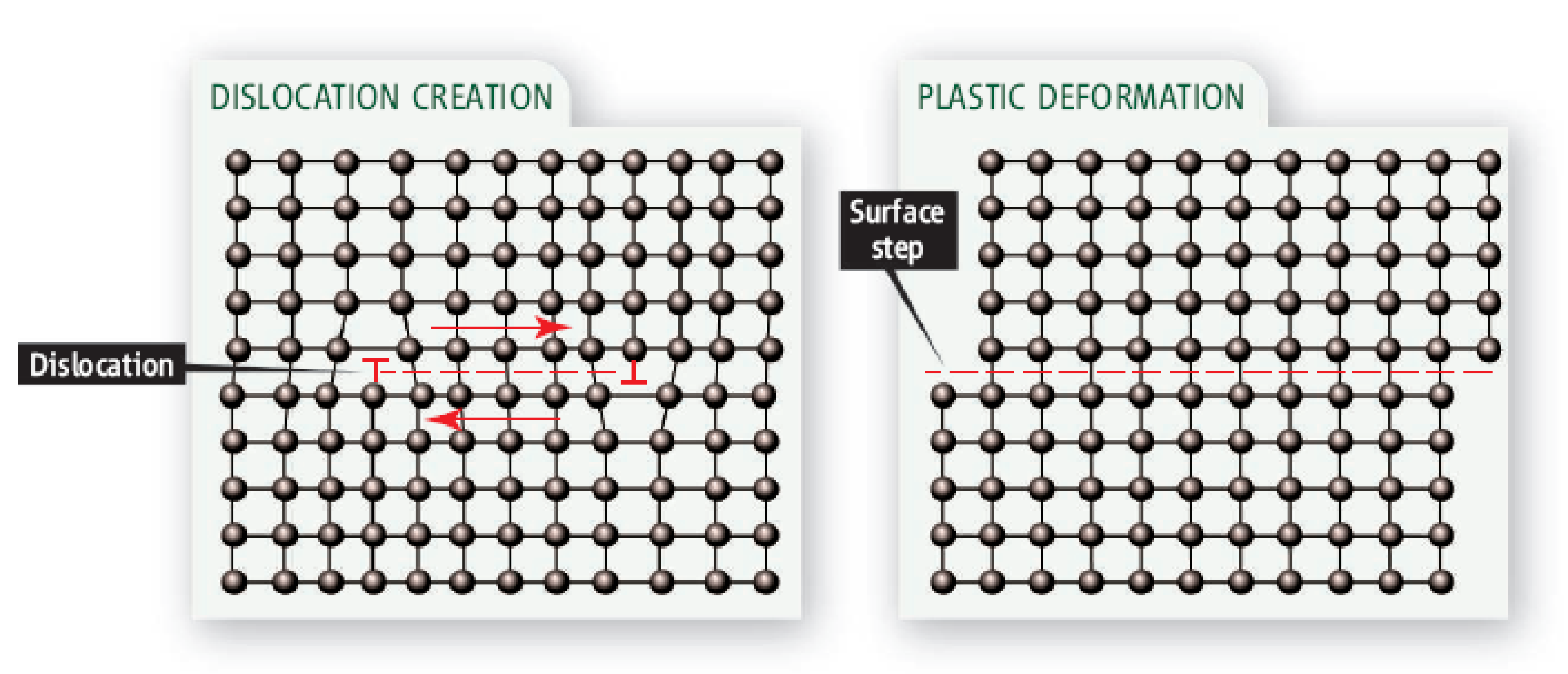
- Turab Lookman, Theoretical Division, Los Alamos National Laboratory

Also see: E. Bouchbinder and J.S. Langer, Phys.Rev. E 80, 031131, 031132, 031133 (2009). (Nonequilibrium thermodynamics)

Plastic Deformation and Dislocations in Crystals



PERSPECTIVES **Anter El-Azab**

SCIENCE VOL 320 27 JUNE 2008

A.H. Cottrell (2002) “Strain hardening [rather than turbulence], is the most difficult remaining problem in classical physics. …. Neither of the two main strategies of theoretical many-body physics -- the statistical mechanical approach; and the reduction of the many-body problem to that of the behaviour of a single element of the assembly -- is available to [strain] hardening. The first fails because the behaviour of the whole system is governed by that of weakest links … and is thermodynamically irreversible. The second fails because dislocations are flexible lines, interlinked and entangled, so that the entire system behaves more like a single object of extreme structural complexity and deformability … a bird's nest … rather than as a set of separate small and simpler elementary bodies.

“[The theory of strain hardening] is still at the stage of being merely interpretive, not predictive. … It may never develop into such a theory.”

Kocks and Mecking (2003): ``An ab initio theory of strain hardening, with a quantitative prediction of the numerical constants, is unlikely to ever be derived even for a specific case, and impossible with any generality.''

These authors advocate what, from a physicist's point of view, is a purely phenomenological approach, based on extensive observations and a search for trends, but with no hope of uncovering fundamental principles that might lead to predictive theories.

Devincre, Hoc and Kubin (2008): ``The present dislocation-based models for strain hardening still have difficulties integrating elementary dislocation properties into a continuum description of bulk crystals or polycrystals. As a consequence, current approaches cannot avoid making use of extensive parameter fitting.''

Intro

Strength can be described by constitutive models such as the new LLNL multiscale models

Ave. disloc. vel.: (MD) $v = \dfrac{M}{\eta b}\dfrac{\dot{\varepsilon}_p}{\rho_d}$,

Flow stress: (continuum) $\sigma_e = M\left[\tau^*(v,\theta)\tau_P(p) + \hat{\tau}(p,\rho) + \tau_a\right]$

Work hardening: (DD) $\hat{\tau}(p,\rho) = \beta b G\sqrt{\rho_d}$,

Peierls stress: $\tau_P = \tau_{P_0}\dfrac{G}{G_0}$

Shear modulus: $G = G(P,T)$

Thermal activation: $\tilde{\tau}_T(v,\theta) = \alpha_0 \exp\left(\dfrac{\theta}{\alpha_T}\right)\left\{\exp\left[\left(\beta_0 + \dfrac{\theta}{\beta_T}\right)\ln\left(\dfrac{v}{c_0} + \tilde{v}_0\right)\right] - \exp\left[\left(\beta_0 + \dfrac{\theta}{\beta_T}\right)\ln(\tilde{v}_0)\right]\right\}$

Phonon drag: $\tilde{\tau}_D(v,\theta) = \max\left\{\left(\dfrac{v}{c_0} - \chi_1\right)\left(\chi_0 + \chi_{0_{\theta 1}}\theta + \chi_{0_{\theta 2}}\theta^2\right)\Big/\sqrt{1 - \left(\dfrac{v}{c_0}\right)^2},\quad 0\right\}$

Combined: $\tau^* = \left(\tilde{\tau}_T^q + \tilde{\tau}_D^q\right)^{1/q}$,

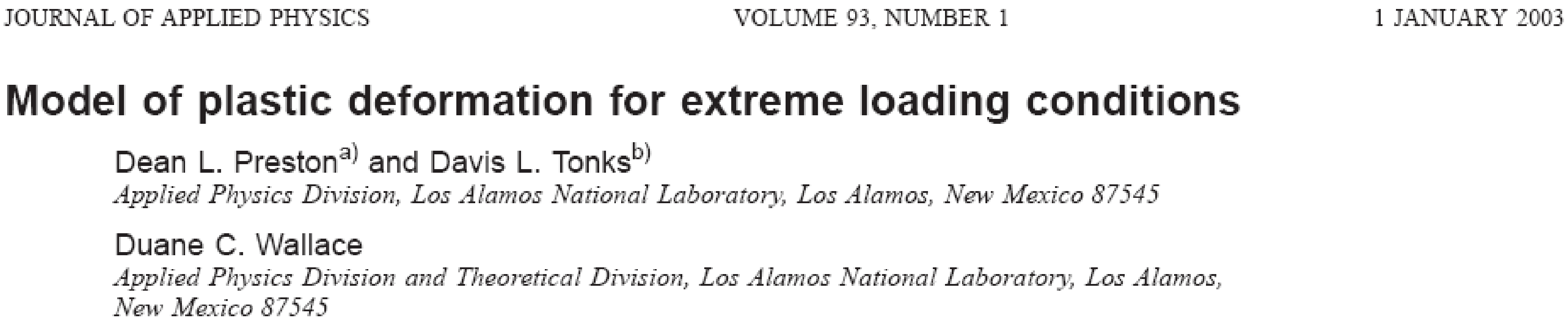
Drag proportion parameter: $f_D = \dfrac{\tilde{\tau}_D^q}{\tilde{\tau}_T^q + \tilde{\tau}_D^q} = 0 - 1$

Disloc. sat. density: $\rho_{sat}(\dot{\varepsilon}_p) = \rho_{s0}\left(\dfrac{\dot{\varepsilon}_p}{\dot{\varepsilon}_N} + S_0\right)^n \sim \rho_{s0}\dot{\varepsilon}_p^n$,

Evolution: $\dot{\rho} = R\left(1 - \dfrac{\rho}{\rho_{sat}(\dot{\varepsilon}_p)}\right)\dot{\varepsilon}_p$

- No twinning, no grain size effects, dislocation density is evolved and is a function of strain rate

[N.R. Barton et al., JAP, 109, 073501 (2011); Barton and Rhee, JAP 114, 123507 (2013)]



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Model of plastic deformation for extreme loading conditions

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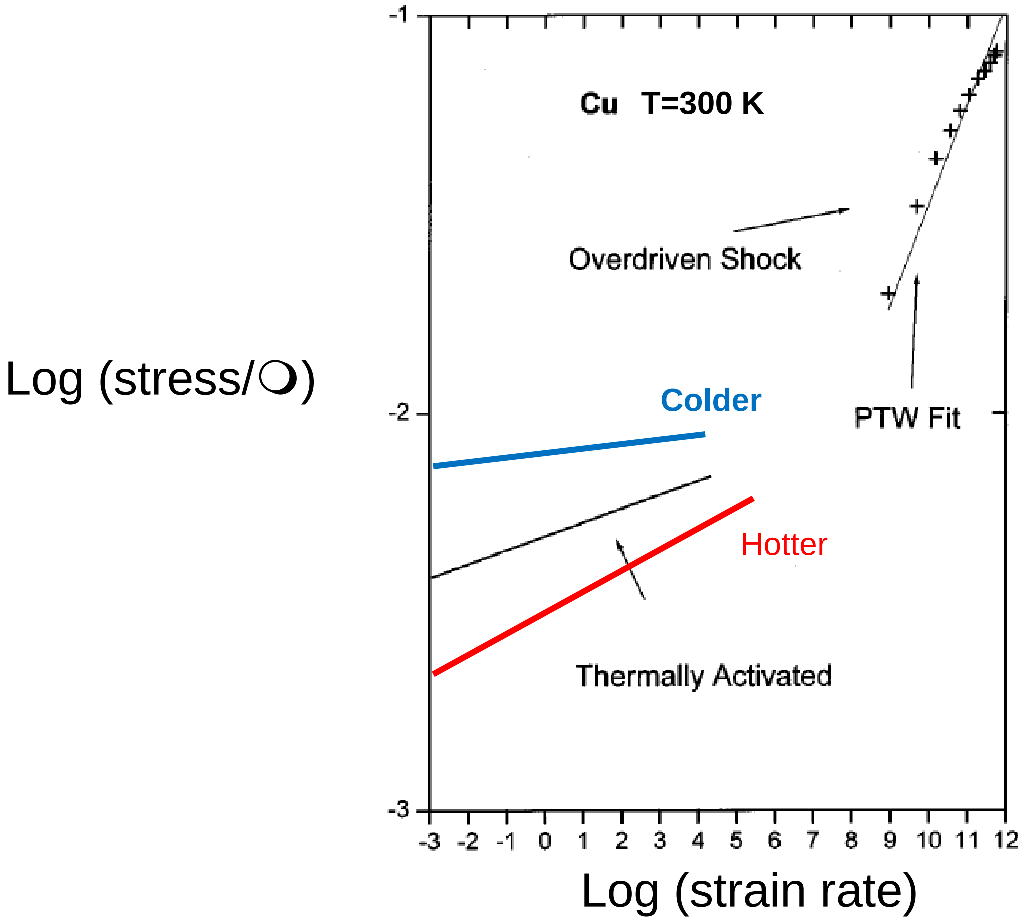
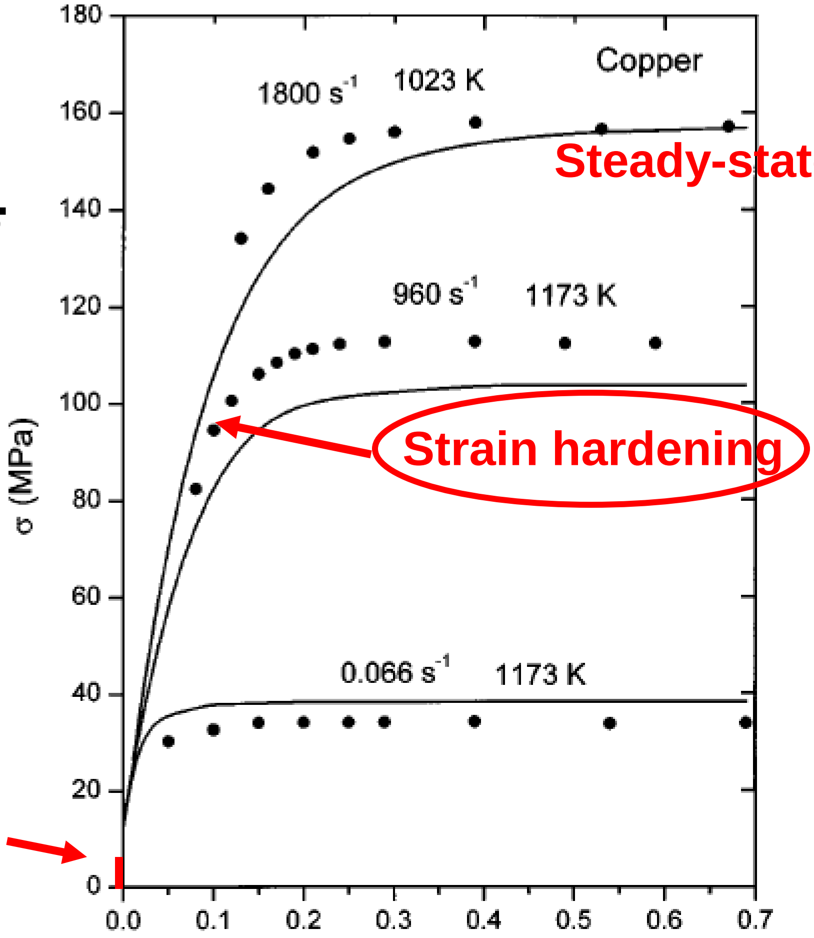


Constant Strain Rate Measurements: Cu at high temperatures



Stress σ (MPa)

Steady-state deformation

Strain hardening

Elastic region

Strain ε

The solid curves are PTW phenomenological fits to a wide range of data.

How can thermodynamics be relevant to dislocations?

Consider only systems that are undergoing persistent deformation in response to external driving forces. The dislocations are moving chaotically. Therefore, we can assume that they are exploring statistically significant fractions of their configuration spaces.

Accordingly, a macroscopically large system of dislocations must be near its state of maximum probability – i.e. maximum entropy – or else it must be moving toward that state.

This system must obey some form of the second law of thermodynamics.

Thermodynamics and dislocations

Dislocation energies are vastly greater than kT. However, The energy U_C of a configuration of dislocations is well defined, and the number of such configurations in an energy interval is countable. Thus, the configurational entropy S_C is also well defined.

The quantity $\chi = \partial U_C / \partial S_C$ is an “effective” temperature. In fact, it is a real temperature.

According to Gibbsian statistical mechanics, the state that minimizes the free energy

$$F_C = U_C - \chi S_C$$

is the most probable state of the sytem.

Steady-State Deformation

Start by considering deformation at fixed shear rate.

ρ = length of dislocations per unit volume. Measure χ in units of some (very large) characteristic energy per dislocation.
F_C is minimized by

$$\rho(\chi) = \frac{1}{a^2} e^{-1/\chi}$$

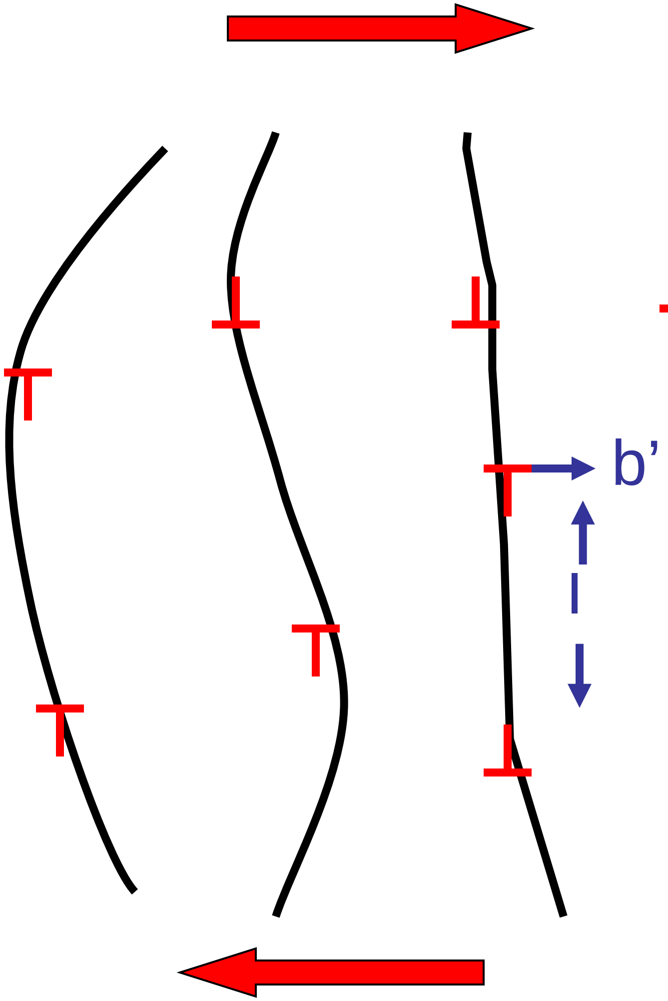
where ***a*** is a length scale (~ 10 lattice spacings ?).

(See B-L 09 for a derivation of this familiar result in a nonequilibrium context.)

To use $\rho(\chi)=\frac{1}{a^2}e^{-1/\chi}$ we need:

(1) An expression for the plastic strain rate $\dot{\varepsilon}^{pl}$ as a function of the stress σ and the dislocation density ρ (a physics-based constitutive law).

(2) A relation between the strain rate and the effective temperature χ (a statistical relation between a steady deformation rate and the state of disorder).



Taylor stress
~ depinning stress

$$\sigma_T = \mu \frac{b'}{\ell} \equiv \mu_T b \sqrt{\rho}$$

b = Burgers vector
~ lattice spacing
b' ~ b/10

(This is fundamentally just dimensional analysis.)

The edge dislocations that produce shear deformation ($\perp$ and $\top$) must move through a "forest" of perpendicular dislocations and other defects that exert pinning forces.

Depinning model of dislocation dynamics

$$\frac{1}{\tau(\sigma)} = \frac{1}{\tau_0} exp\left[-\frac{U(\sigma)}{k_B T}\right]$$

= thermally activated
depinning rate

$\tau_0 \approx 10^{-12}$ sec.

For arbitrarily large σ, write the depinning barrier in the form

$$U(\sigma) = k_B T_P\, exp\left[-\frac{\sigma}{\sigma_T(\rho)}\right]$$

This is the *simplest possible* smooth function with only one stress scale, chosen here to be the Taylor stress.

Assume that a dislocation spends almost all of its time in a pinned state, and occasionally jumps instantaneously from one such state to another. Then, after some dimensional analysis *a la* Orowan, the dimensionless plastic strain rate *q* turns out to be:

$$q(\sigma,\rho) \equiv \dot{\varepsilon}^{pl}\tau_0 = b\,\tau_0\sqrt{\rho}\left[\frac{1}{\tau(\sigma)} - \frac{1}{\tau(-\sigma)}\right]$$

We already have some important information. For all but very small stresses σ, we can drop the – σ term in the formula for *q*(*σ*,ρ), and solve for (positive) σ as a function of *q* and ρ:

$$\frac{\sigma}{\sigma_T(\rho)} = ln\left(\frac{T_P}{T}\right) - ln\left[\frac{1}{2} ln\left(\frac{b^2\rho}{q^2}\right)\right]$$

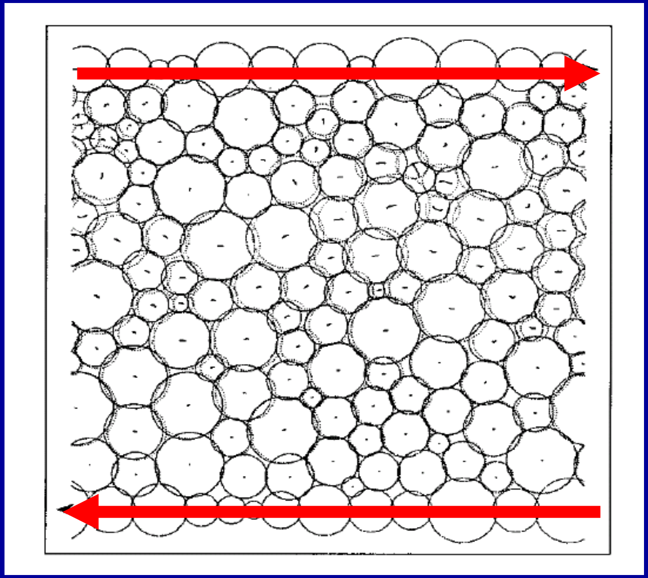
Note the double logarithm.

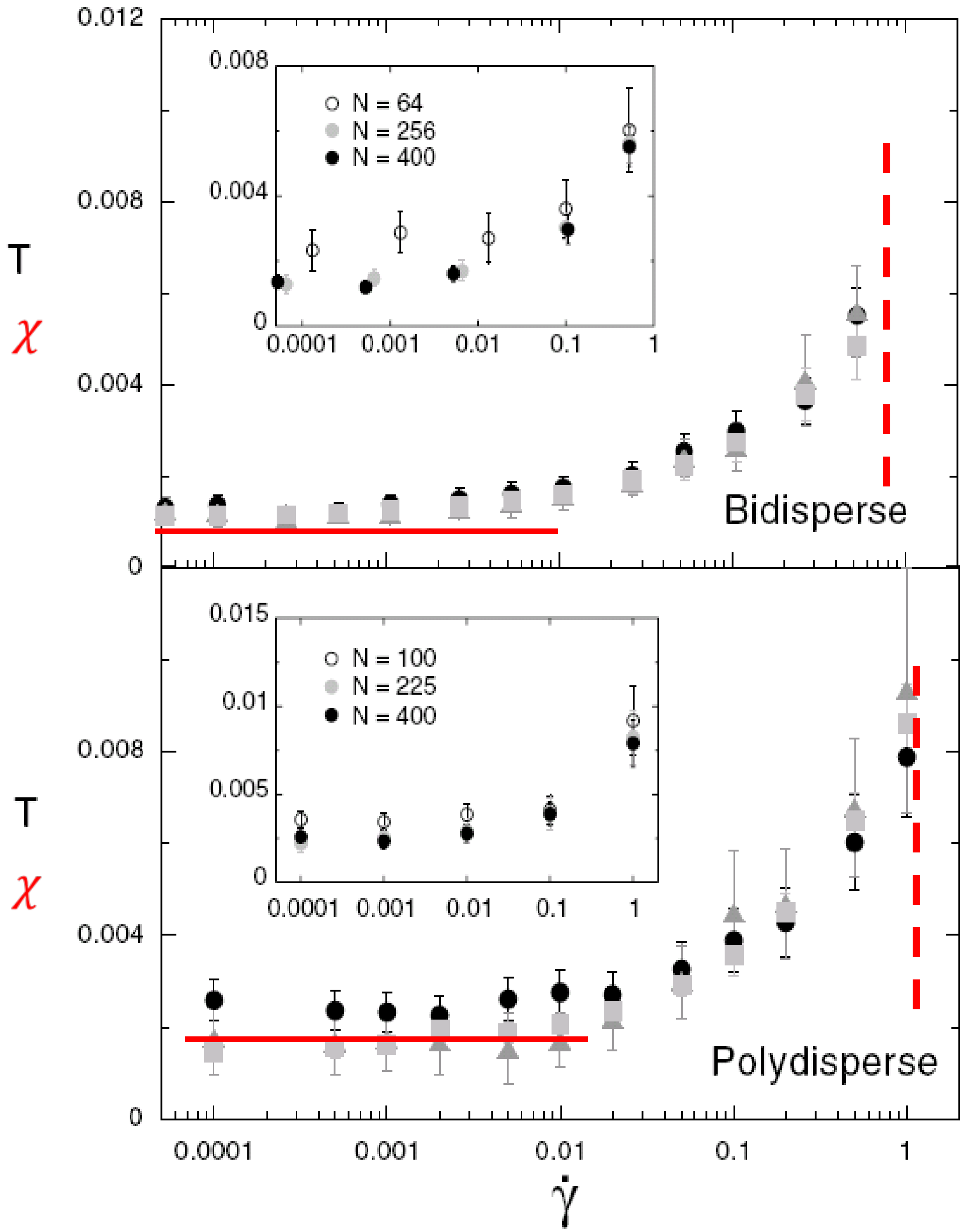
So long as the strain rate is almost entirely plastic, the stress is proportional to the Taylor stress, and the proportionality factor is an extremely slowly varying function of its arguments.

This is the physics-based constitutive relation that we need.

We next need a relation between the deformation rate and the state of disorder specified by the effective temperature χ.

Borrow an idea from nonequilibrium theories of amorphous materials, in this case, numerical simulations of a sheared foam by Ono et al. The basic idea is that shearing is like “stirring,” and that stirring produces disorder.





Sheared Foam

Ono, O'Hern, Durian, (S.) Langer, Liu, and Nagel, PRL 095703 (2002)

Temperature, measured in several different ways (response-fluctuation theorems, etc.), goes to a nonzero constant in the limit of vanishing shear rate.

$$\chi \to \chi_0$$

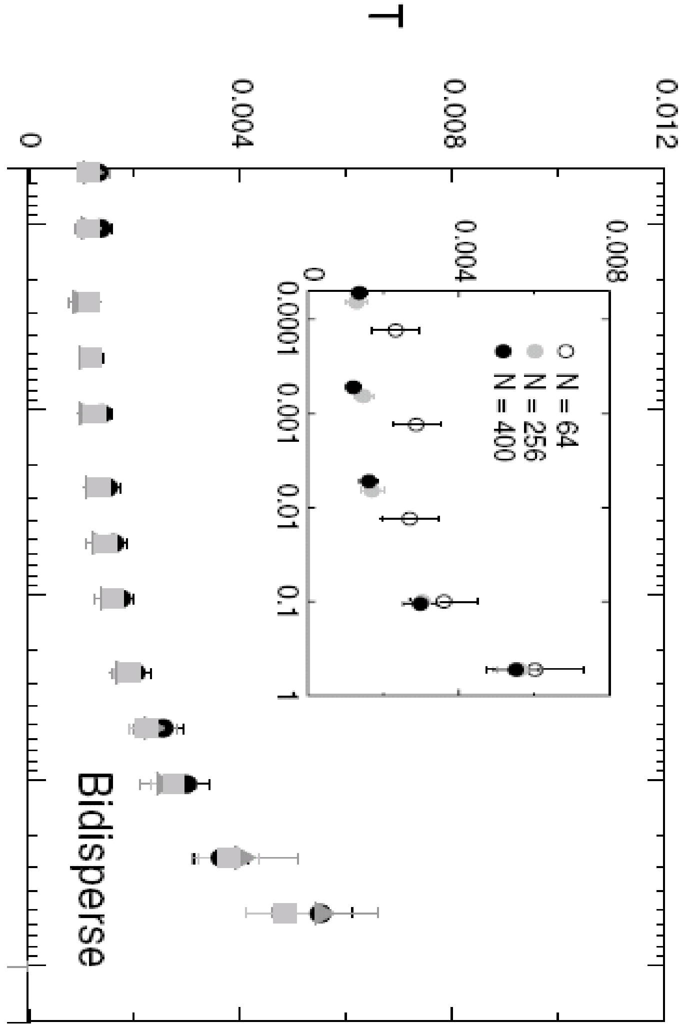
More generally, as seen in the graphs,

$$\chi \to \hat{\chi}\left(\dot{\gamma}^{pl}\right)$$

which apparently diverges at a large but finite strain rate.

Rotate graph of effective temperature versus strain rate

$1/\dot{\gamma} \sim \tau_\alpha \sim \eta$



$T \sim \chi$

The dimensionless strain rate is $q = \dot{\varepsilon}^{pl} \tau_0$
where, as before, τ_0 is a microscopic time scale.

$$\chi(q) \rightarrow \chi_0,\; q << 1$$

("glass transition")

$$\chi(q) \approx -\frac{A}{\ln q},\; q \cong 1; \quad \Rightarrow \; q \approx e^{-A/\chi}$$

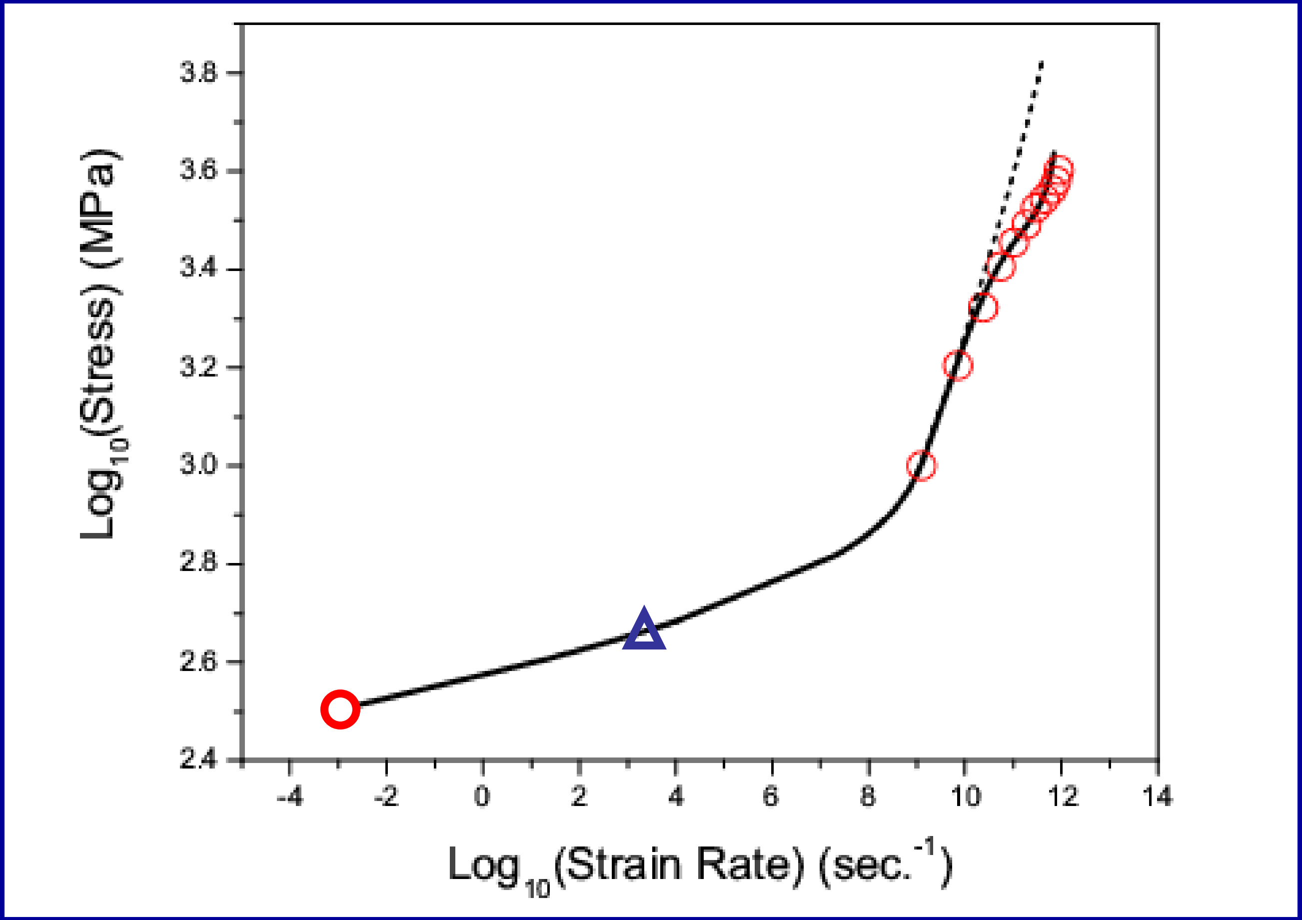
("Arrhenius region")

Then $$\rho(\chi) = \frac{1}{a^2} e^{-1/\chi}$$

becomes an expression for $\rho(q)$. Finally

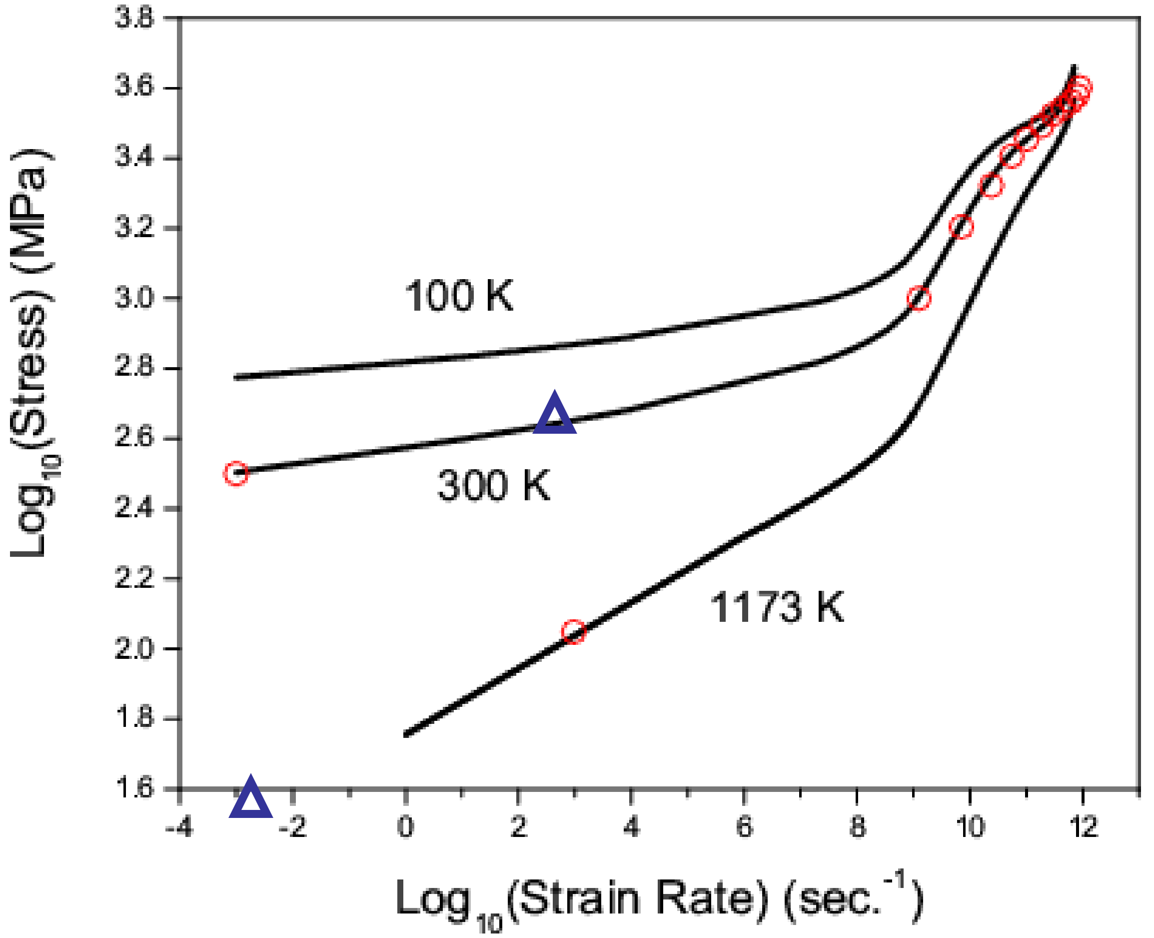
$$\frac{\sigma}{\sigma_T(\rho)} = \ln\left(\frac{T_P}{T}\right) - \ln\left[\frac{1}{2}\ln\left(\frac{b^2\rho}{q^2}\right)\right]; \quad \sigma_T(\rho) = \mu_T b\sqrt{\rho}$$

gives us the stress – strain-rate relation $\sigma(q)$.



Steady-state stress versus strain rate for Cu at T = 300K. The two points at smaller strain rates are steady-state limits of selected laboratory experiments. The fall-off at the highest strain rates is fit by a heating effect.

Main idea --- the rapid growth of ♍(q) as q→1 rapidly increases the density of dislocations and, accordingly, increases the stress.



Same stress versus strain rate curve as in previous graph, but also showing higher and lower temperatures.

Steady-State Parameters

$\tau_0 = 10^{-12}\ sec$	Molecular vibration period
$\chi_0 = 0.25$	From observed dislocation densities
$T_P = 40{,}800\ K$	Pinning energy ~ 3eV
$\mu_T = \mu / 31$	❍(T) = shear modulus ~ 50 GPa at 300 K
$A = 2$	Fits both upper slope and crossover between low and high strain rates.

These are the *only* parameters needed in the steady-state theory, except for a thermal transport coefficient used to describe the heating effect at the highest strain rates.

Strain-Hardening Theory

The crucial ingredients are equations of motion for χ and ρ that describe the way these quantities approach their steady-state equilibrium values as functions of time or total strain. These equations are:

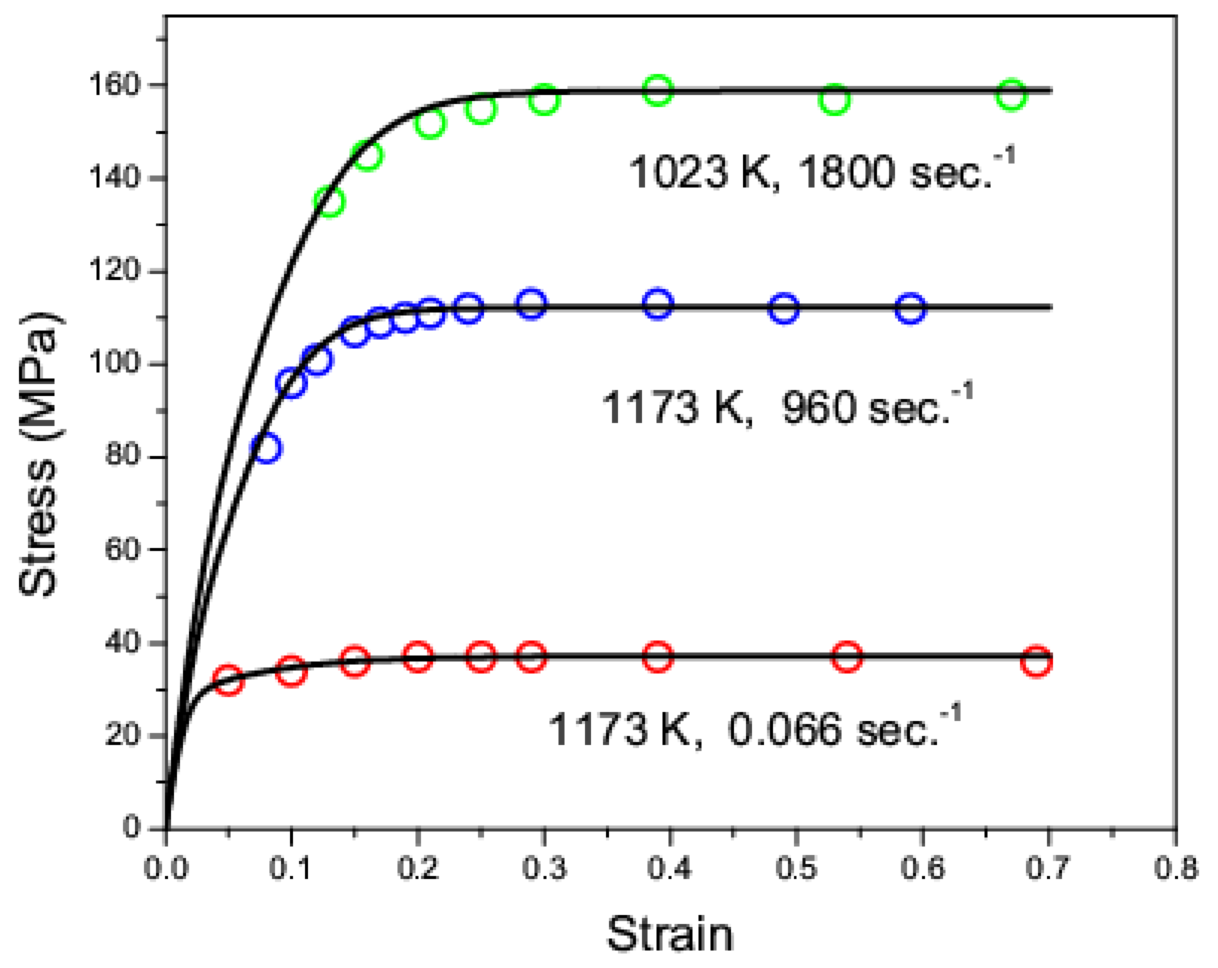
$$c^{eff}\,\dot{\chi} = \kappa\,\dot{\varepsilon}^{pl}\,\sigma\left(1-\frac{\chi}{\chi_0}\right)$$

Entropy flow (first law of thermodynamics)

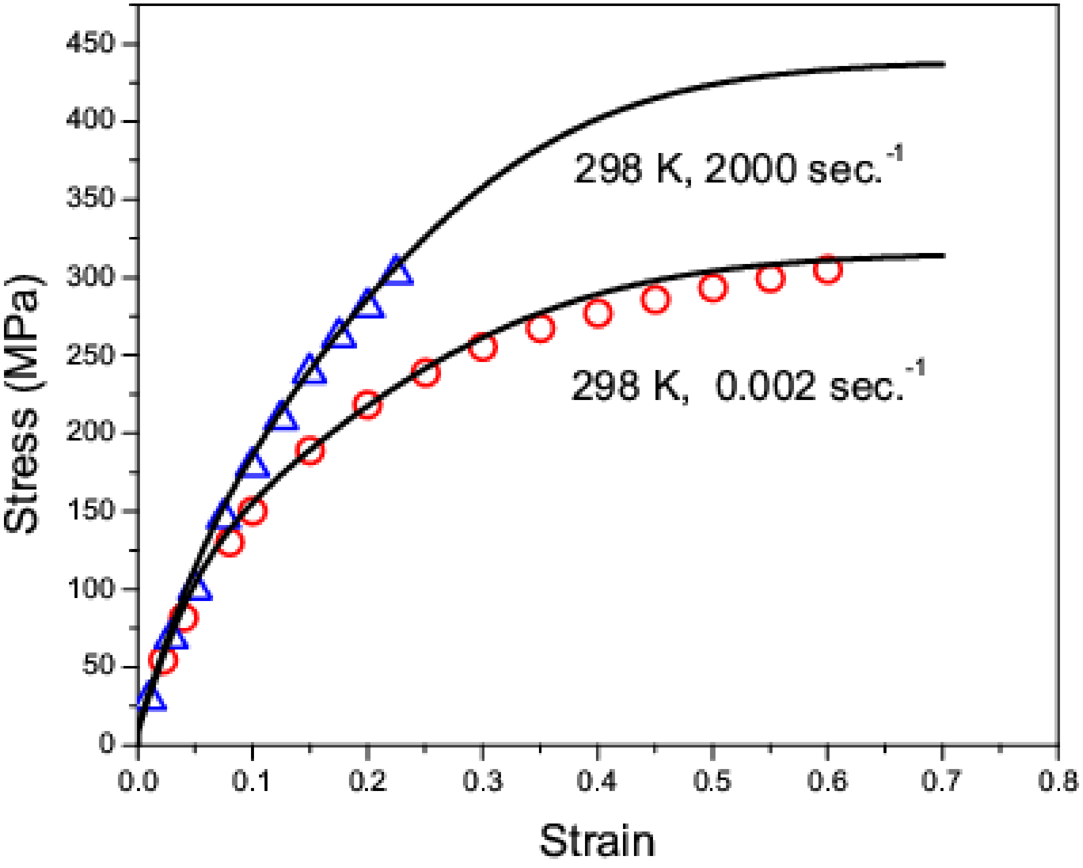
$$\dot{\rho} = \kappa_\rho\,\frac{\dot{\varepsilon}^{pl}\,\sigma}{\gamma_D}\left[1-\frac{\rho}{\rho^{eq}(\chi)}\right]; \qquad \rho^{eq}(\chi) = \frac{1}{a^2}\,e^{-1/\chi}$$

Energy conservation

γ_D = dislocation energy per unit length. The κ's are dimensionless proportionality factors. Note that both rates are determined by the rate at which work is done on the system by the applied stress σ.



Stress-strain curves for copper at high temperatures, for constant (shear) strain rates as shown. The theoretical curves are from JSL et al.



Stress-strain curves for copper at about room temperature, for constant, very different, (shear) strain rates as shown. The theoretical curves are from JSL et al.

Heresies

- The principles of nonequilibrium thermodynamics are relevant to dislocation-mediated plasticity.

- There is no useful distinction between “stored” and “mobile” dislocations.

- The Kocks-Mecking equation for the dislocation density is incorrect; it violates fundamental physical principles. It can be replaced by a simple statement of energy conservation.

- In most nonequilibrium situations, the speed at which a dislocation moves from one pinning site to another is irrelevant; only the depinning rate makes a difference.

Unsolved, Probably Solvable Problems

- Include elastic energy explicitly.
- Onset of hardening.
- Dynamic origin of cellular dislocation patterns.
- Dynamics of shear banding and shear fracture.
  (Is dynamic recrystallization an entropic effect? Is it the relevant softening mechanism?)