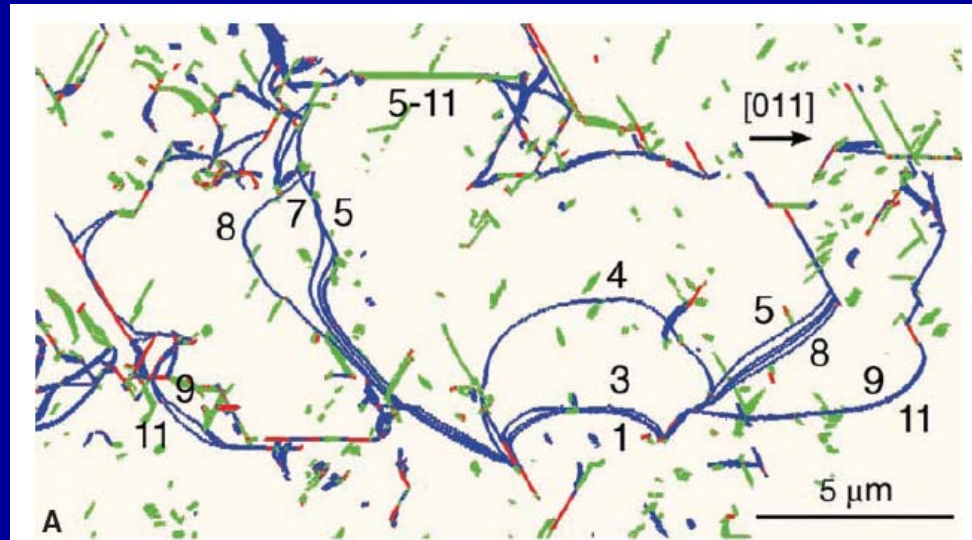


Thermodynamics of Solid Plasticity: The Effective Temperature of Dislocations



J.S. Langer
KITP Glass Conference
June 24, 2010

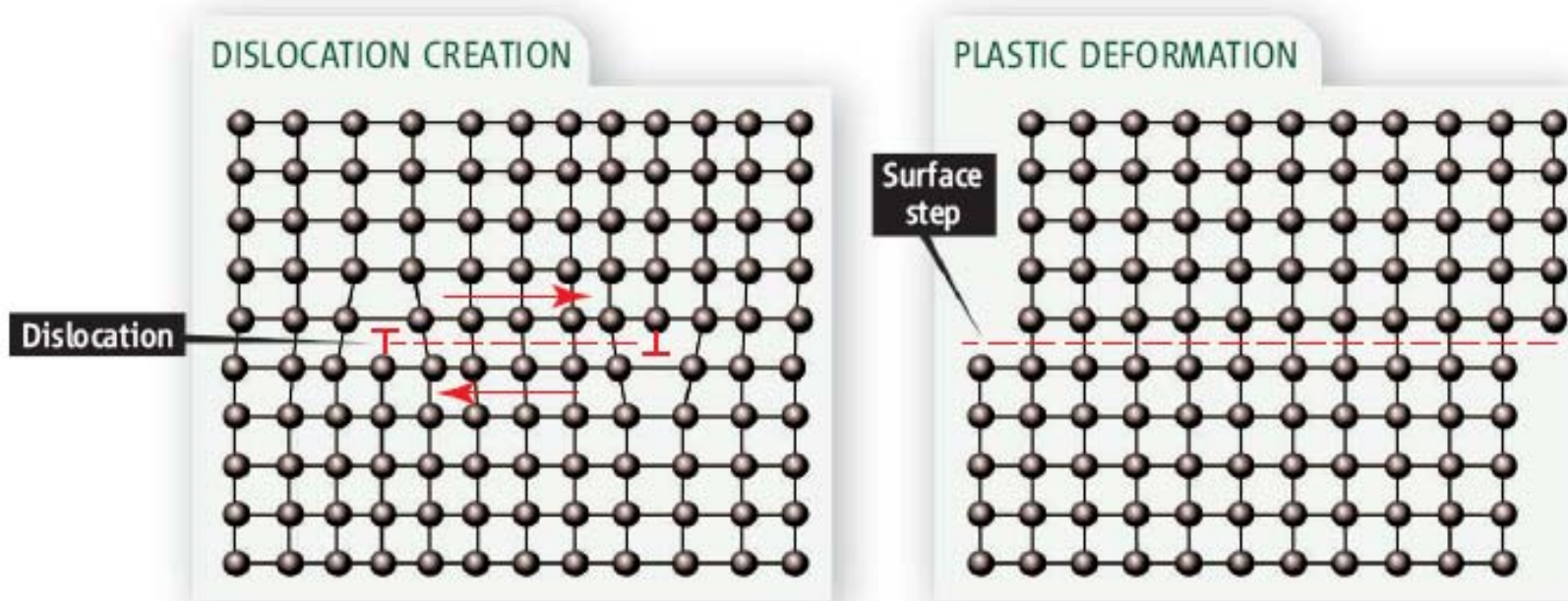
Thermodynamic theory of dislocation-mediated plasticity, *Acta Materialia* 58, 3718 (2010)

- J.S. Langer, Physics Department, University of California, Santa Barbara
- Eran Bouchbinder, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel
- 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)

E. Bouchbinder and J.S. Langer, *Soft Matter* 6, 3065 (2010) (Kovacs effect)

Plastic Deformation and Dislocations in Crystals



PERSPECTIVES **Anter El-Azab**

SCIENCE VOL 320 27 JUNE 2008

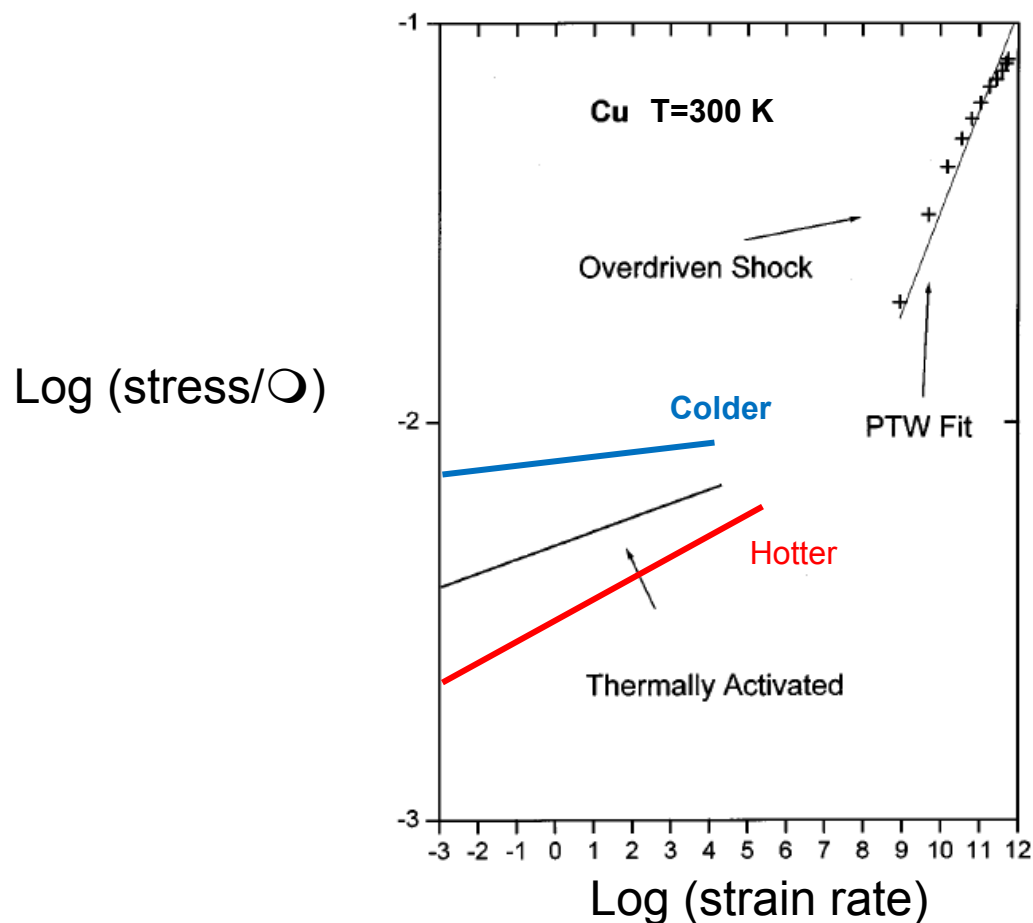
Model of plastic deformation for extreme loading conditions

Dean L. Preston^{a)} and Davis L. Tonks^{b)}

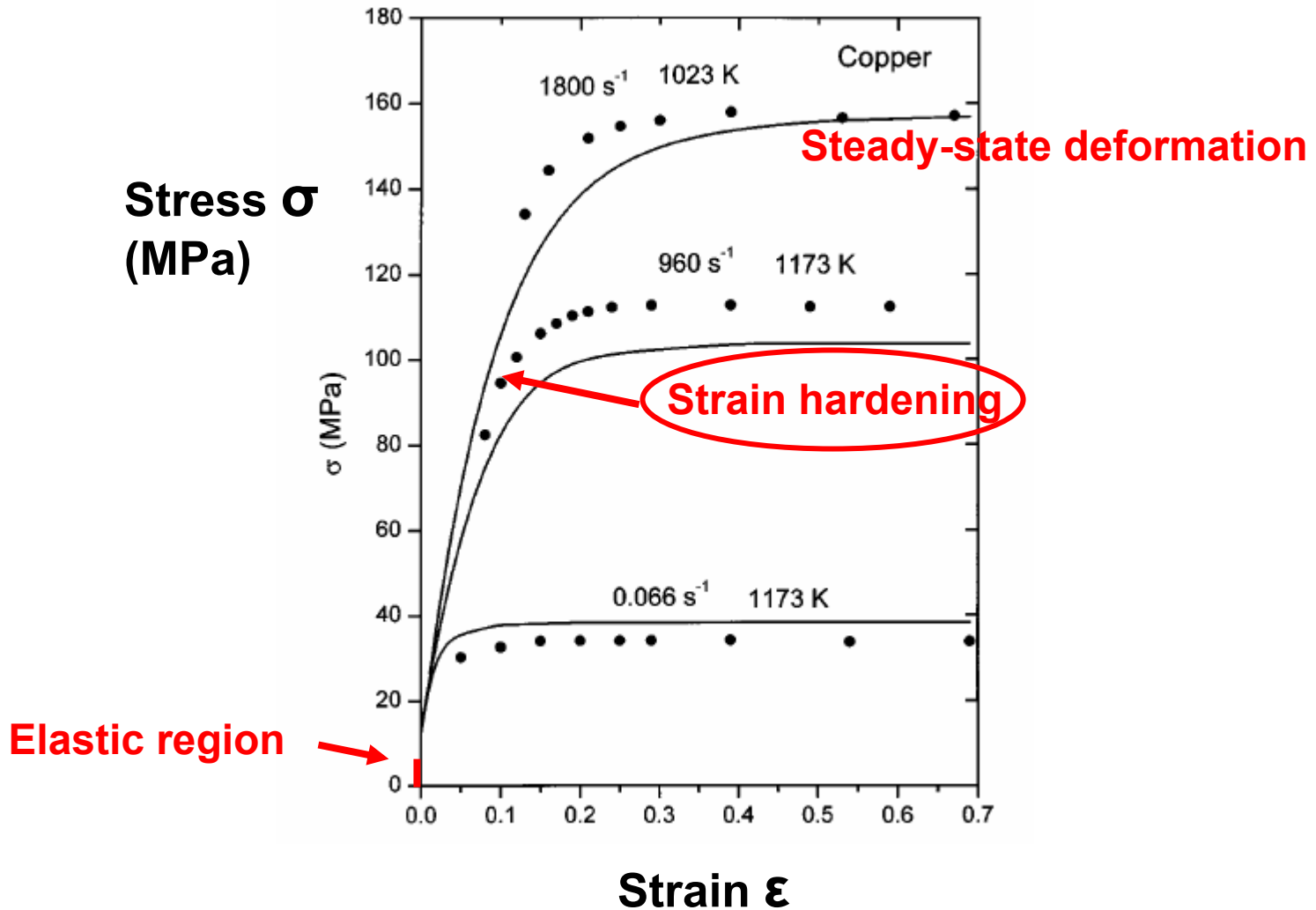
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Constant Strain Rate Measurements: Cu at high temperatures



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

A.H. Cottrell (2002) “Strain hardening [rather than turbulence], is the most difficult remaining problem in classical physics.

“[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.”

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.”

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 system.

Steady-State Deformation

Start by considering deformation at fixed shear rate.

ρ = number of dislocations per unit area. Measure \mathcal{M} in units of some (very large) characteristic energy per dislocation.

F_C is minimized by

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

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 $\dot{\epsilon}^{pl}$ 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 \mathfrak{M} (a statistical relation between a steady deformation rate and the state of disorder).

Computational Dislocation Dynamics

B. Devincere,¹ T. Hoc,² L. Kubin^{1*}

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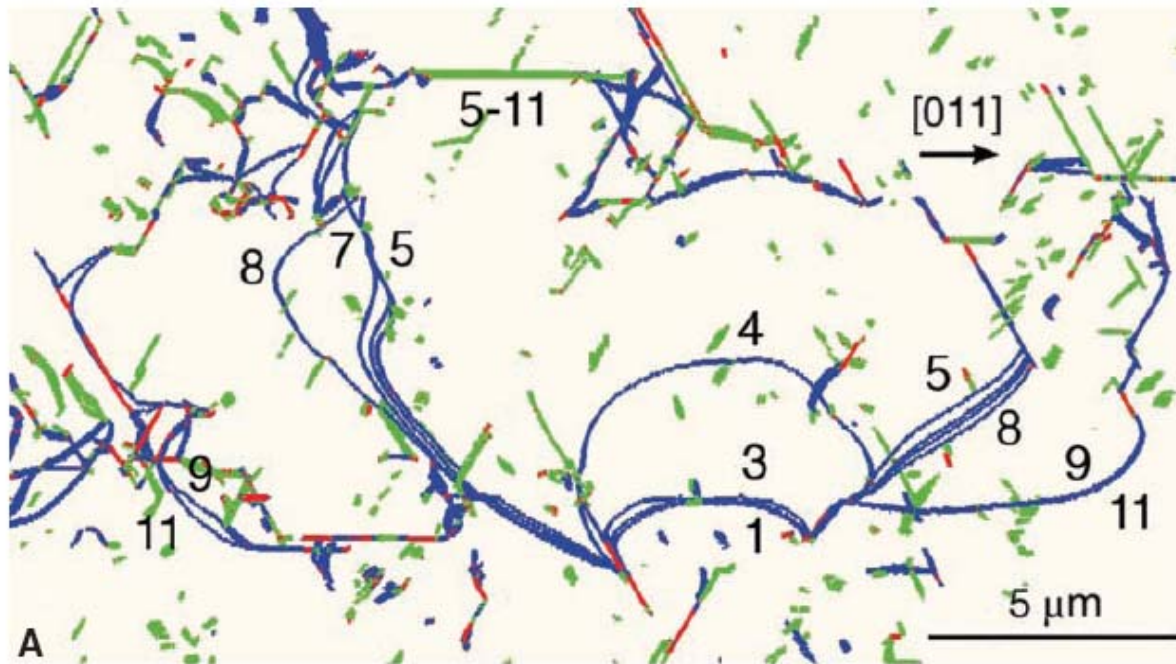
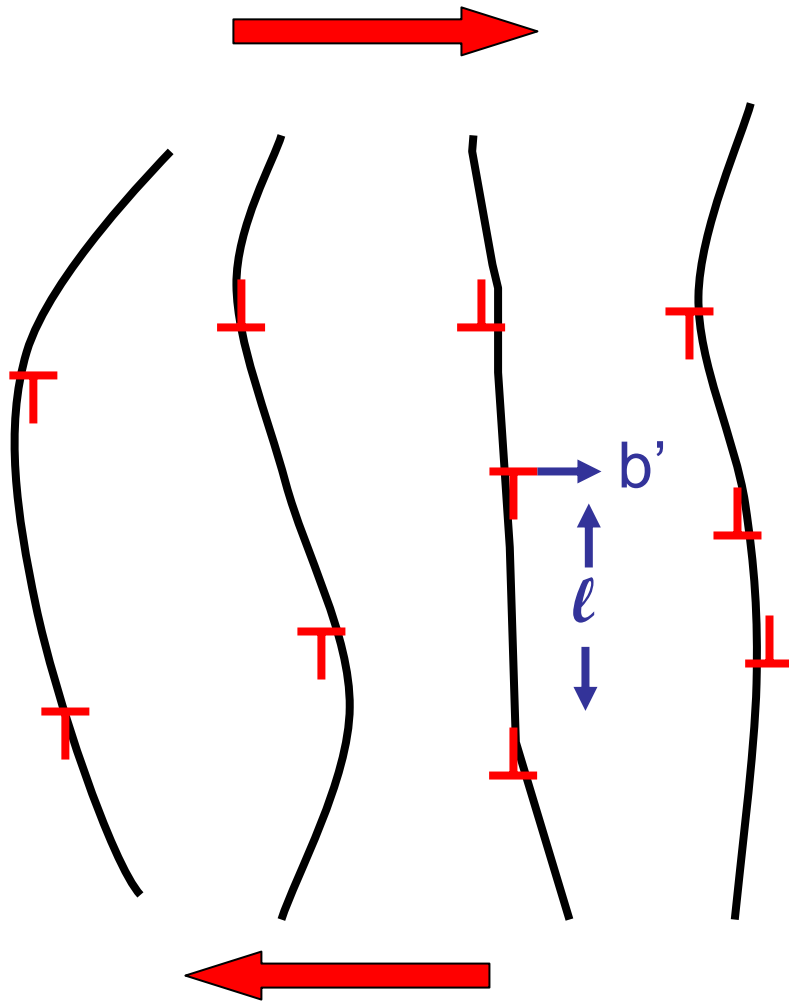


Fig. 1. Strain bursts during large-scale DD simulations of tensile deformation in copper crystals. The elementary simulation cell has a size of 4.4-by-4.9-by-5.9- μm^3 , the imposed strain rate is 10 s^{-1} , and periodic boundary conditions were used (4). (A) Successive dislocation avalanches occurring in the slip system $s = [011](\bar{1}\bar{1}1)$ of a deforming $[001]$ crystal. Superimposed configurations taken at constant time intervals are shown in a thin film of thickness = $0.25 \mu\text{m}$ containing the active set of $(\bar{1}\bar{1}1)$ extended slip planes. The forest slip systems (short green lines) form junctions (red straight lines) with the active slip system (blue lines). During its expansion, the unpinned segment (1) sweeps an area of $\sim 130 \mu\text{m}^2$ before being stored again at dense forest tangles. (B) Corresponding evolutions of the resolved stress (τ) and dislocation density (ρ) in s versus the total shear strain (γ_p). Each jerk results from an avalanche, and arrow



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

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

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:

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

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

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

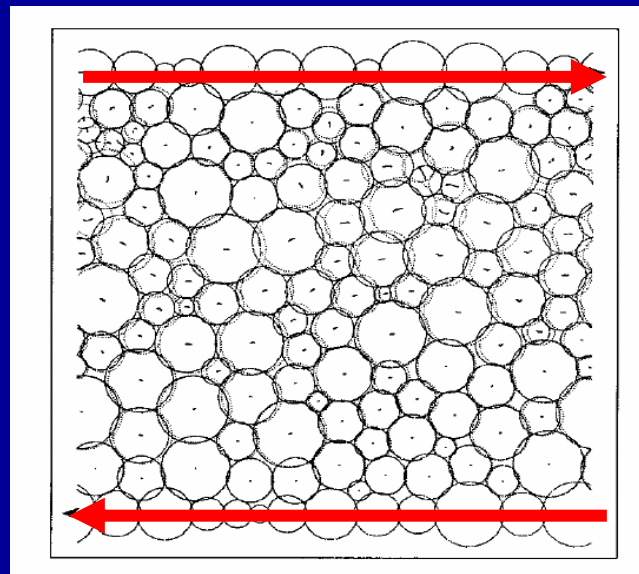
Note the double logarithm.

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 T_{eff} .

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)

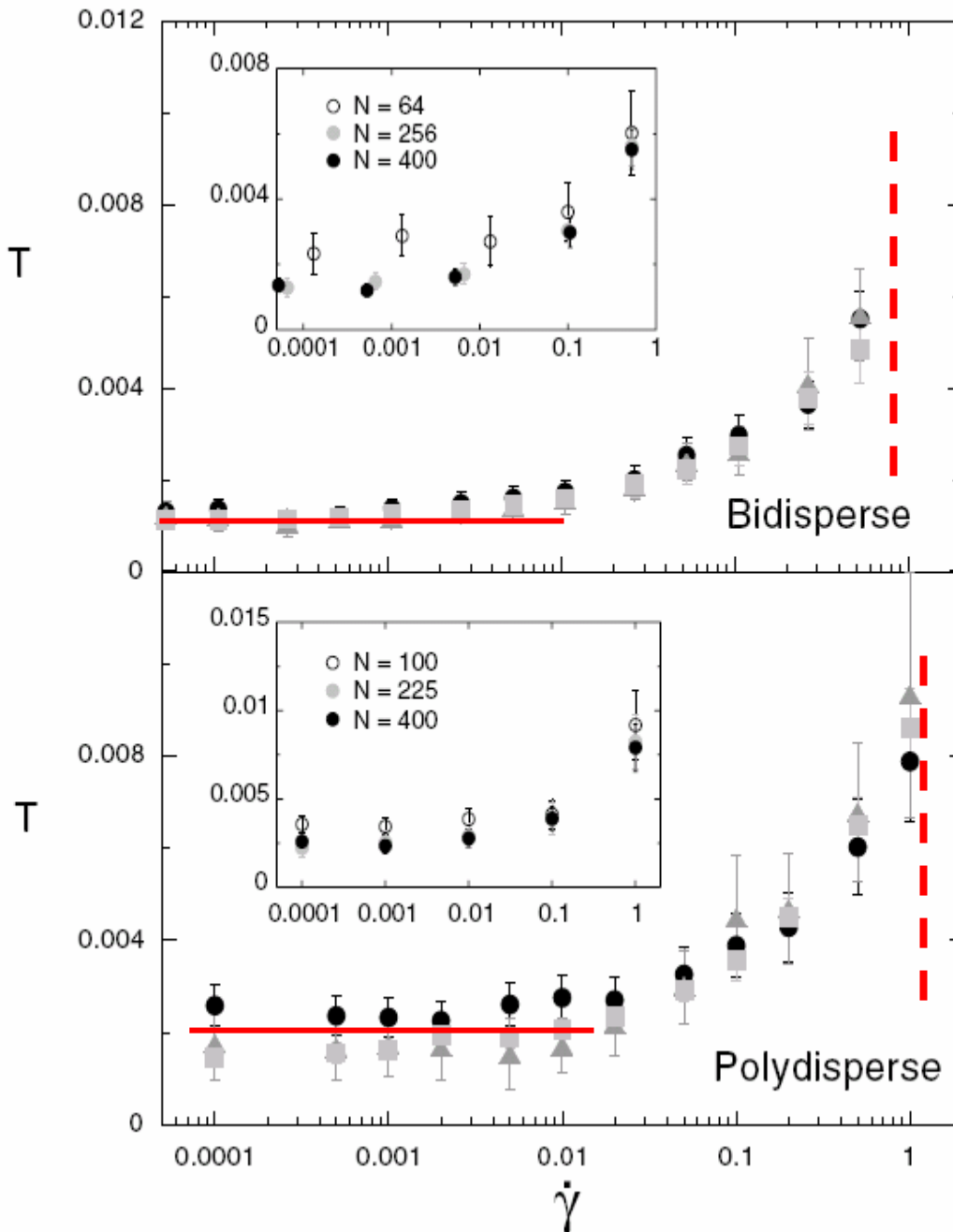
Temperature, measured in several different ways (response-fluctuation theorems, etc.), goes to a nonzero constant in the limit of vanishing shear rate.

$$\chi \rightarrow \chi_0$$

More generally, as seen in the graphs,

$$\chi \rightarrow \hat{\chi}(\dot{\gamma}^{pl})$$

which apparently diverges at a large but finite strain rate.



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

$$\chi(q) \rightarrow \chi_0, \quad q \ll 1$$

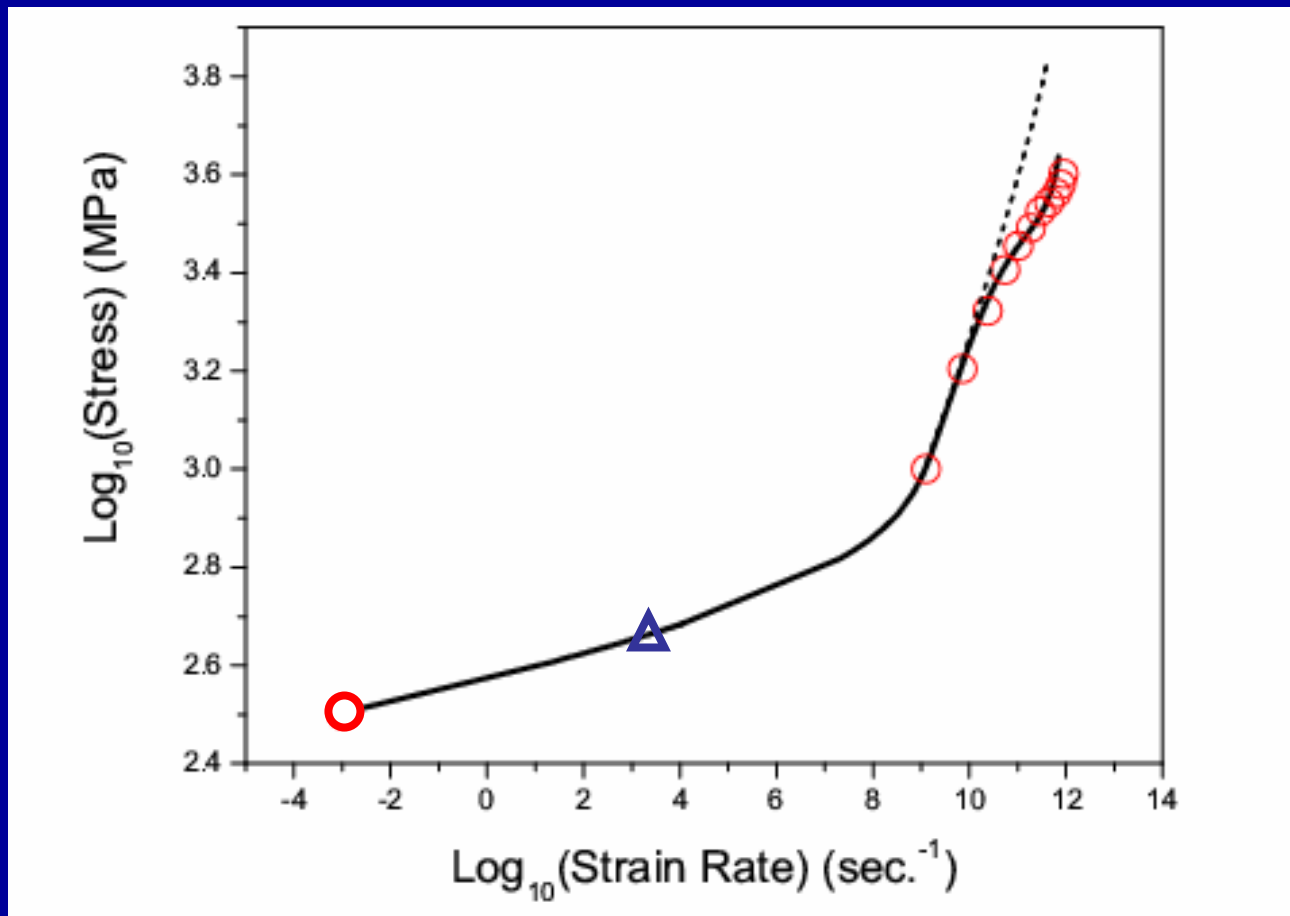
$$\chi(q) \approx -\frac{A}{\ln q}, \quad q \cong 1; \quad \Rightarrow \quad q \approx e^{-A/\chi} \quad (\text{which has a glass-physics interpretation})$$

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 $T = 300\text{K}$. 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 $\mathfrak{M}(q)$ as $q \rightarrow 1$ rapidly increases the density of dislocations and, accordingly, increases the stress.

Steady-State Parameters

$$\tau_0 = 10^{-12} \text{ sec}$$

Molecular vibration period

$$\chi_0 = 0.25$$

From observed dislocation densities

$$T_p = 40,800 \text{ K}$$

Pinning energy $\sim 3\text{eV}$

$$\mu_T = \mu / 31$$

$\circ(T)$ = shear modulus $\sim 50 \text{ GPa}$ 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.

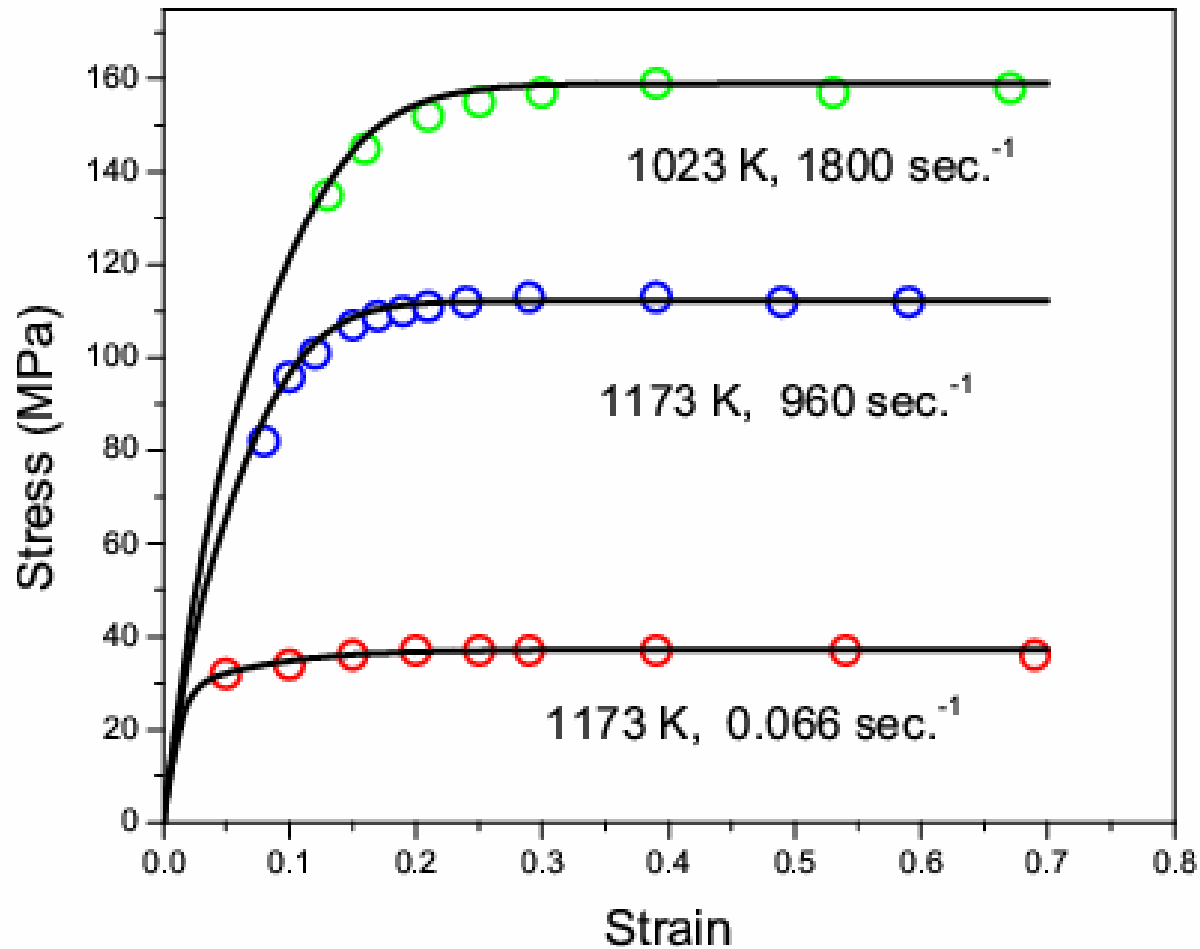
Strain-Hardening Theory

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

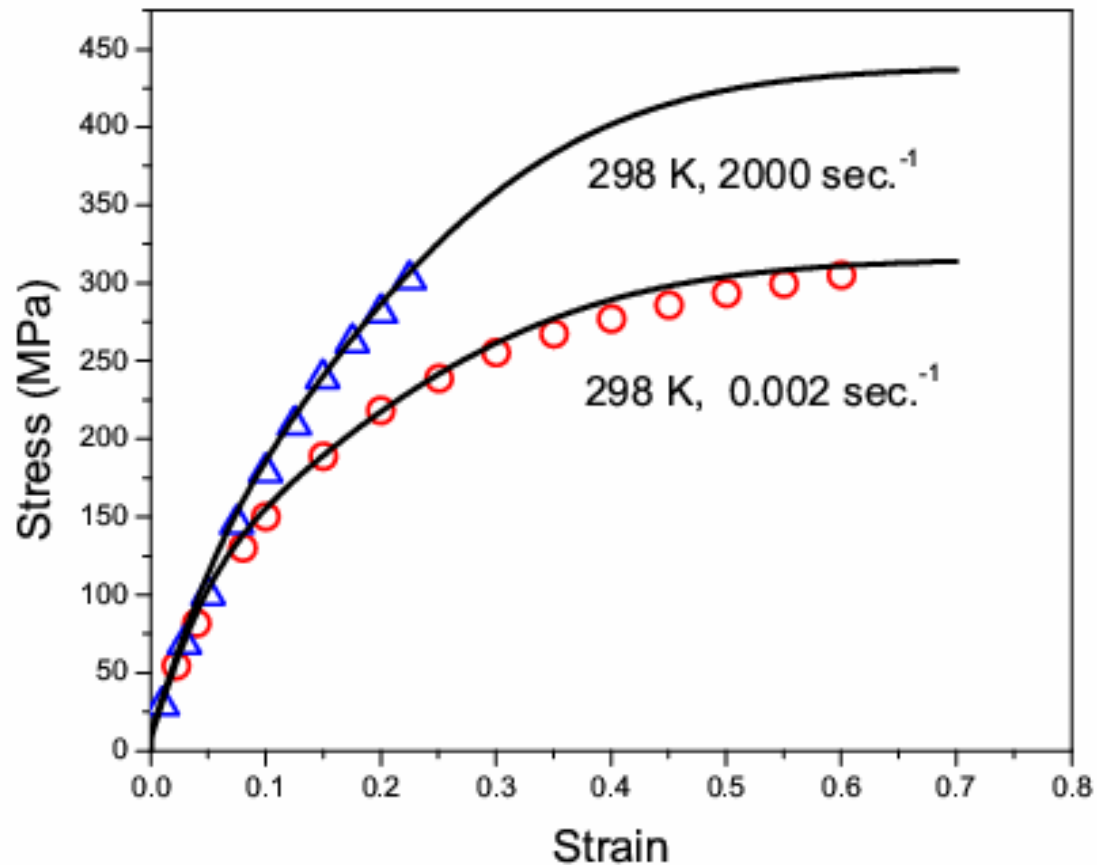
$$c^{eff} \dot{\chi} = \kappa \dot{\epsilon}^{pl} \sigma \left(1 - \frac{\chi}{\chi_0} \right) \quad \text{Entropy flow (first law of thermodynamics)}$$

$$\dot{\rho} = \kappa_{\rho} \frac{\dot{\epsilon}^{pl} \sigma}{\gamma_D} \left[1 - \frac{\rho}{\rho^{eq}(\chi)} \right]; \quad \rho^{eq}(\chi) = \frac{1}{a^2} e^{-1/\chi} \quad \text{Energy conservation}$$

γ_D = dislocation energy per unit length. The K '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 irrelevant; 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.

Unsolved, Probably Solvable Problems

- 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?)

A Broader Perspective

In deforming solids, configurational degrees of freedom undergo chaotic (ergodic) motions. They fall out of equilibrium with the bath temperature, and are naturally described by *effective temperatures*.

A dynamic theory of such systems consists of equations of motion for properly defined internal state variables – i.e. coarse-grained functions of space and time. In crystalline solids, these fields are densities of different kinds of dislocations with varying orientations. This set of fields has been approximated here by a single scalar, areal density ρ .

In amorphous solids, we need a scalar density of flow defects, and a deviatoric tensor field m to determine their average orientation. To describe a broader range of phenomena, including soft glassy rheology, we may need to include a distribution of thermal activation energies associated with the shear transformations.