

Nonequilibrium Thermodynamics of Dislocation-Enabled Plasticity

KITP

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J.S. Langer
U. C. Santa Barbara

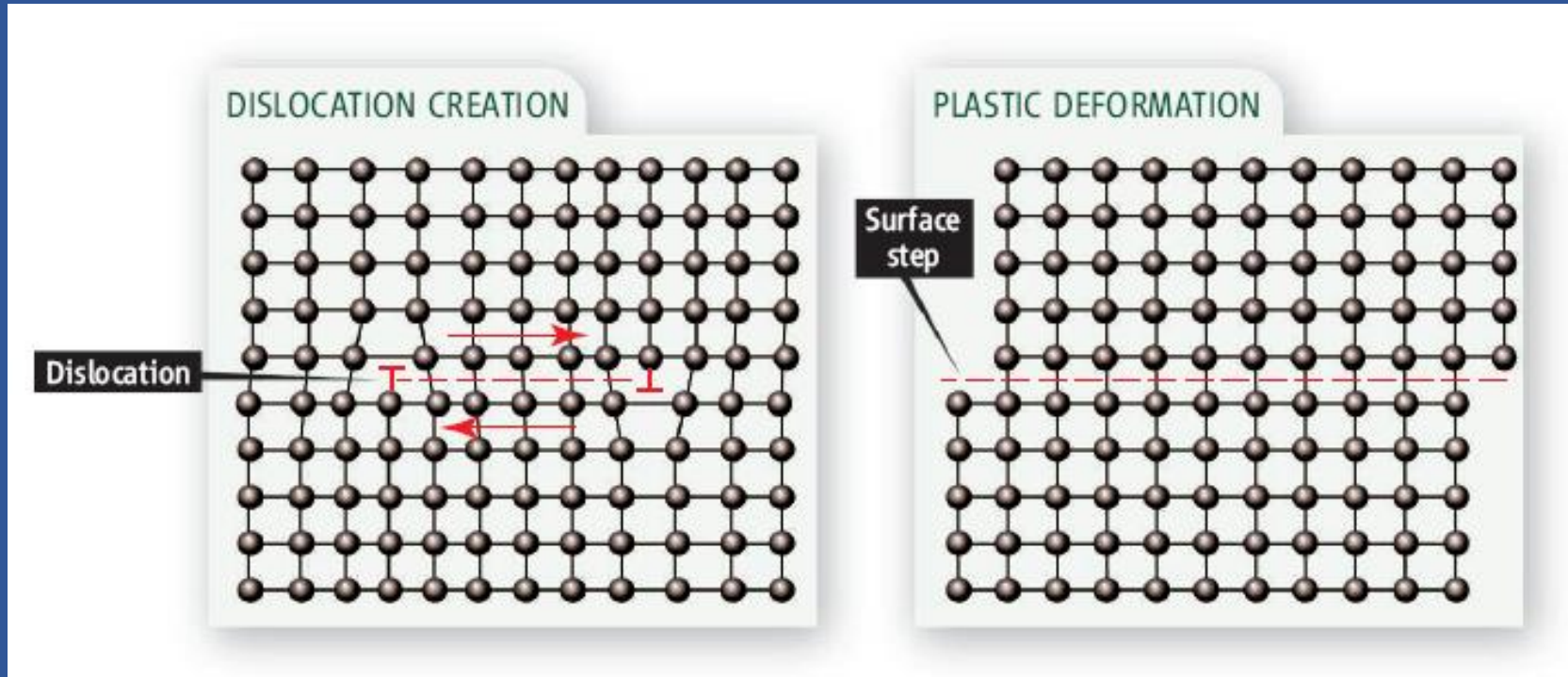
Recent Publications

JSL, E. Bouchbinder, T. Lookman, Acta Mater. 2010 (LBL)

JSL, PRE 2015 – 2017

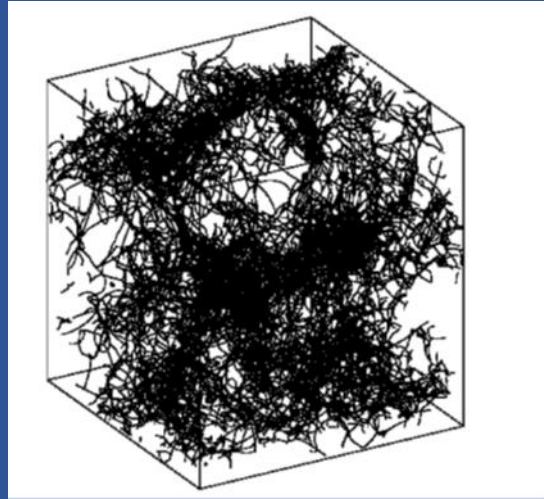
K.C. Le, T.M. Tran, JSL PRE 2017

Plastic Deformation and Dislocations in Crystals



Edge dislocations: Line defects oriented perpendicular to the plane

Dislocations and Strain Hardening



A “bird’s nest” of dislocations
(Nabarro)

Real dislocations are extended line defects in crystals. Their chaotic motions determine irreversible deformations. New dislocations are created by externally applied stresses during strain. They become entangled with each other and, at increasing densities, require increasing stresses to make them move. Thus the material becomes harder and stronger as it deforms.

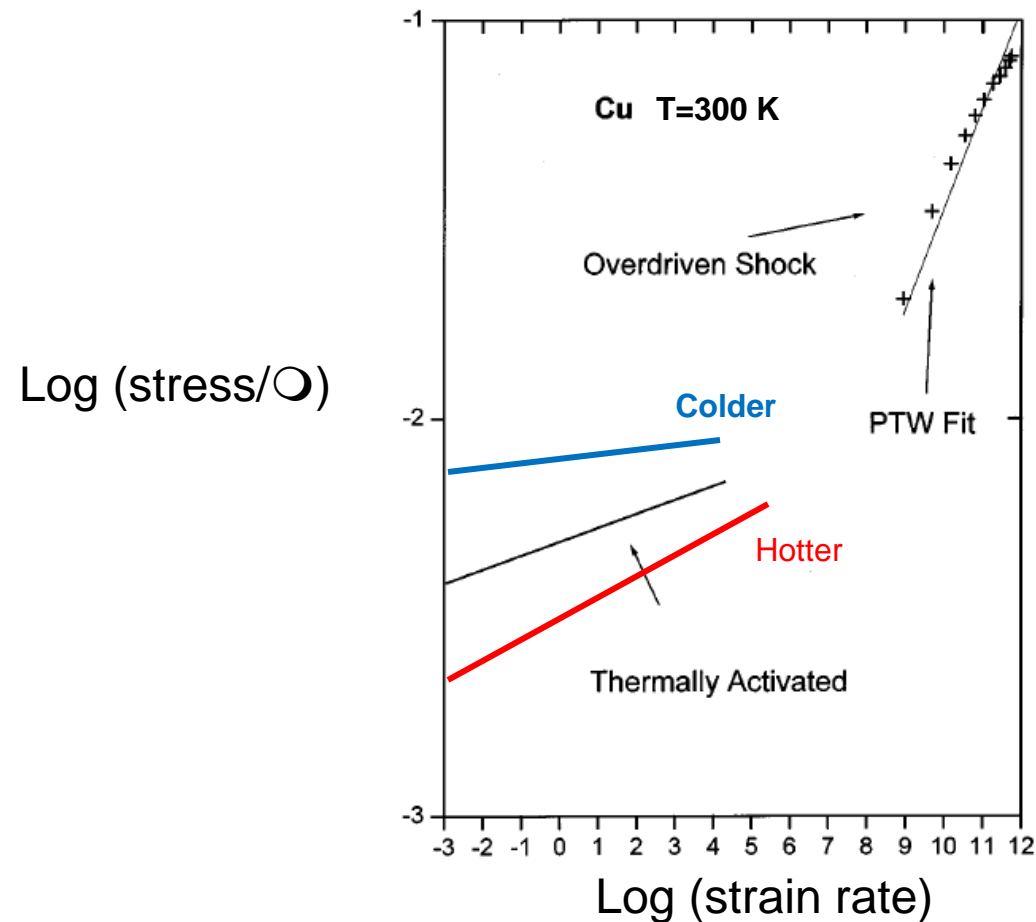
Model of plastic deformation for extreme loading conditions

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

Applied Physics Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

Duane C. Wallace

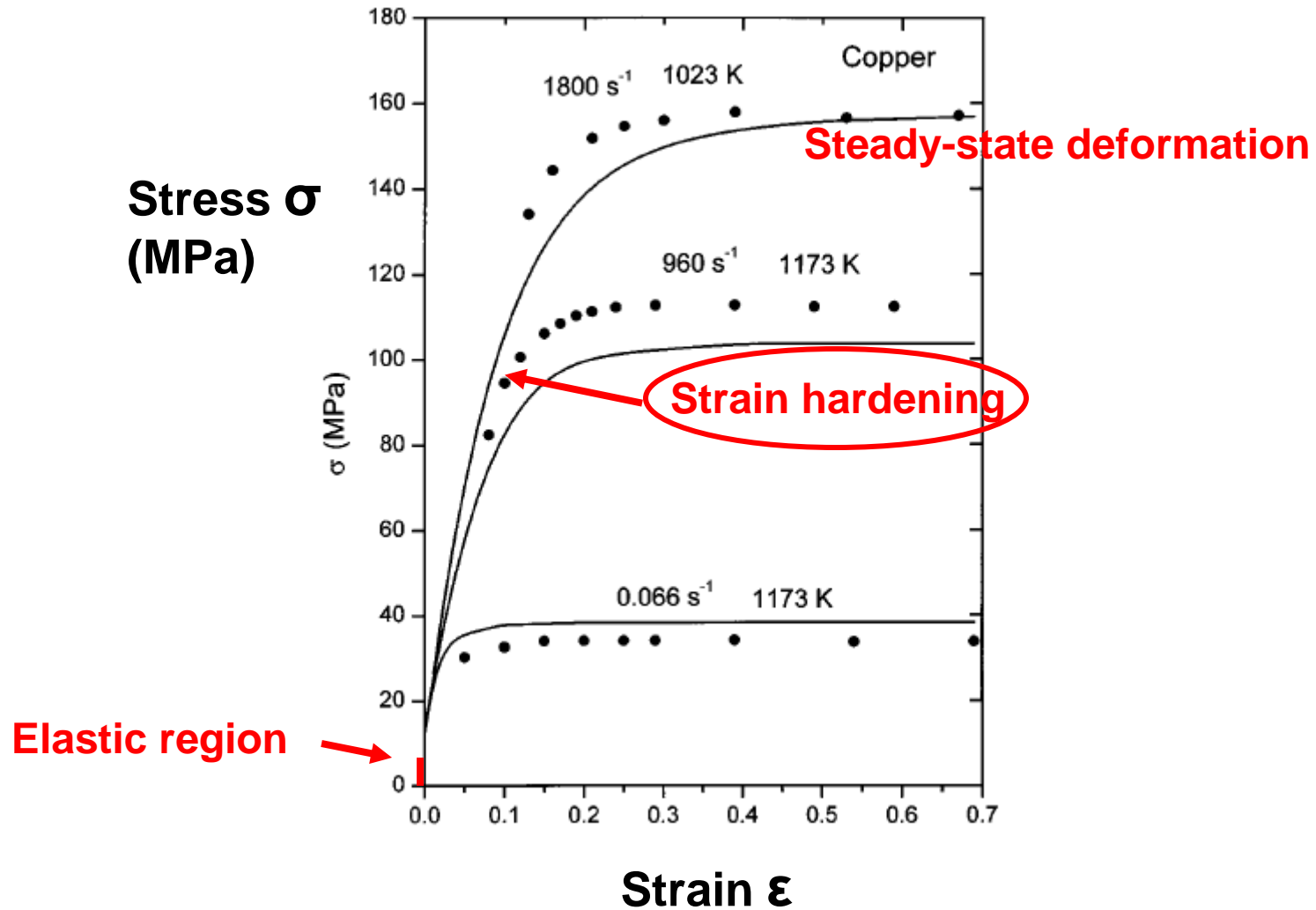
Applied Physics Division and Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545



Note extremely slow variation of stress with strain rate.

Constant Strain Rate Measurements: Cu at high temperatures

Preston, Tonks and Wallace, LANL 2003



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

A.H. Cottrell (2002) In a volume of essays celebrating the 50'th anniversary of his 1952 book on dislocation theory:

“Strain hardening is the most difficult remaining problem in classical physics. The statistical mechanical approach ... fails because the behaviour of the whole system is governed by that of weakest links ... and is **thermodynamically irreversible**. ... The entire system behaves more like a single object of extreme structural complexity and deformability ... a bird's nest.

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

Statistical Thermodynamics of Dislocations

Consider systems that are undergoing persistent deformation in response to external driving forces. The dislocations are moving very slowly on atomic time scales; but they 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 (sub-) system must obey some form of the second law of thermodynamics.

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.

Maximize S_C at fixed U_C , that is, minimize the free energy

$$F_C = U_C - \chi S_C$$

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

When the system is driven out of equilibrium, χ is very different from the ambient temperature. It is a measure of configurational disorder. **It is an essential, memory-carrying, dynamical variable.**

Steady-State Deformation

Measure the effective disorder temperature χ in units of some (very large) characteristic dislocation energy. Minimizing the free energy tells us that the steady-state density of dislocations is:

$$\rho_{ss} = \frac{1}{a^2} e^{-1/\chi_{ss}}$$

where a is a length scale of the order of about 10 lattice spacings, and χ_{ss} is a function of the deformation (“stirring”) rate, but only for very large rates.

For rates slower than atomic relaxation rates, $\chi_{ss} \rightarrow \chi_0 = \text{constant}$.

If ρ is the principal determinant of stress, then we understand why stress is almost constant. An argument analogous to the Lindemann criterion for melting implies that $\chi_0 \cong 0.25$, which is close to the observed value.

Deformation Rates

Start with **Orowan's relation** (1930's)

ρ = density of dislocations per unit area
= length of dislocation lines per unit volume $\approx \frac{1}{\ell}$

ℓ = average spacing between dislocations

Plastic shear rate $\dot{\epsilon}^{pl} = \rho v b$

where v = average velocity of dislocations
 b = length of Burgers vector \sim atomic spacing

G. I. Taylor (1934)

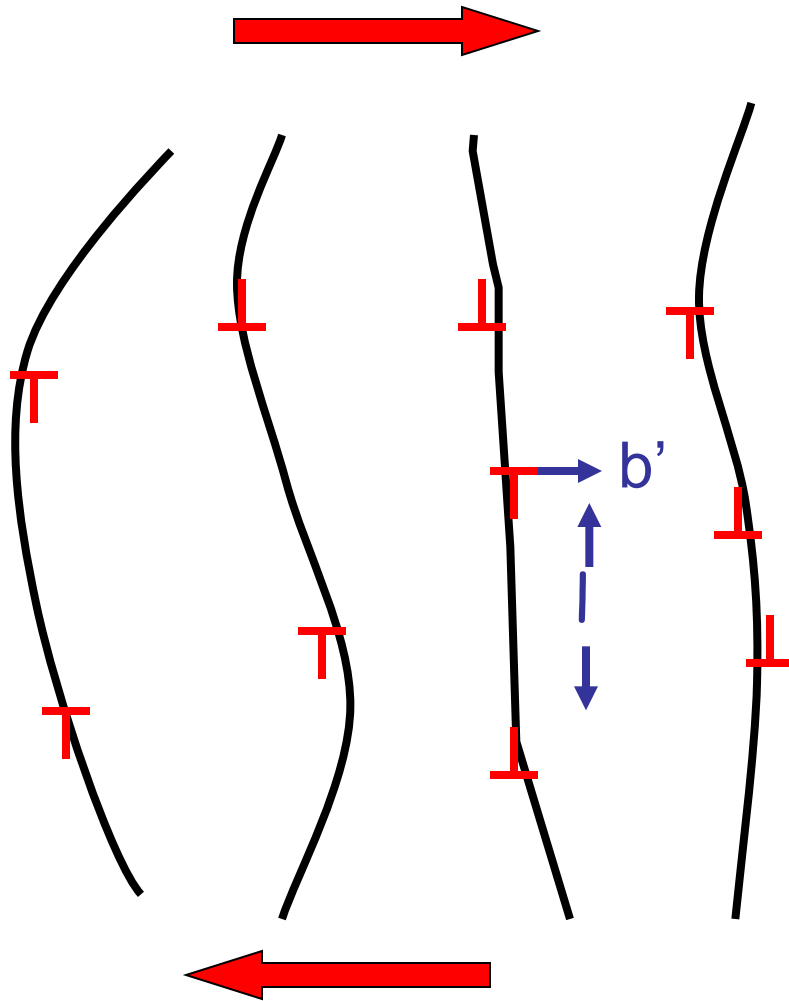
(more or less)

Taylor stress:

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

b = Burgers vector
~ lattice spacing

b' ~ b/10



The edge dislocations that produce shear deformation (**L** and **T**) must move through a “forest” of perpendicular dislocations and other defects that exert pinning forces.

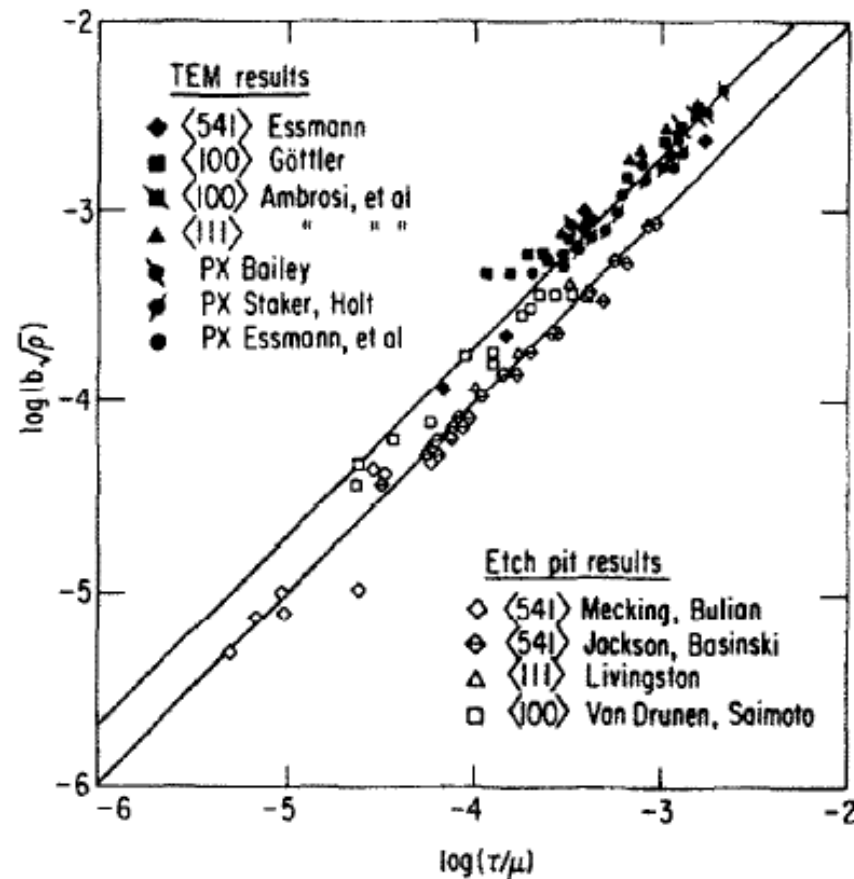


Fig. 1. Dislocation density vs flow stress for Cu at room temperature [12-21], normalized by $b = 0.256$ nm, $\mu = 42.1$ GPa (decadic logarithms). Polycrystal (PX) tensile stresses were divided by 3.06 to convert to shear stress τ . Volume dislocation densities measured by TEM were divided by 2 to convert to intersection density ρ . For single slip $\langle 541 \rangle$, etch-pit data refer to forest density, TEM data to dislocations with nonprimary Burgers vectors. From the low stresses, 0.12 MPa was subtracted [20]. The lines show the relation $\sigma = \alpha \mu b \sqrt{\rho}$, with $\alpha = 1$ and 0.5.

Depinning model

$$\frac{1}{\tau(\sigma)} = \frac{1}{\tau_0} \exp\left[-\frac{\Delta E(\sigma)}{k_B T}\right] \quad \text{thermally activated depinning rate}$$

$$\Delta E(\sigma) = k_B T_P \exp\left[-\frac{\sigma}{\sigma_T(\rho)}\right] \quad \tau_0 = 10^{-12} \text{ sec. (microscopic time scale)}$$

$\Delta E(\sigma)$ is just a convenient smooth function with only one stress scale, i.e. the Taylor stress. Assume (correctly) that a dislocation spends almost all of its time in a pinned state, and occasionally jumps almost instantaneously from one such state to another. Then, use the Orowan relation with $v = \ell / \tau(\sigma)$ to evaluate the dimensionless plastic strain rate :

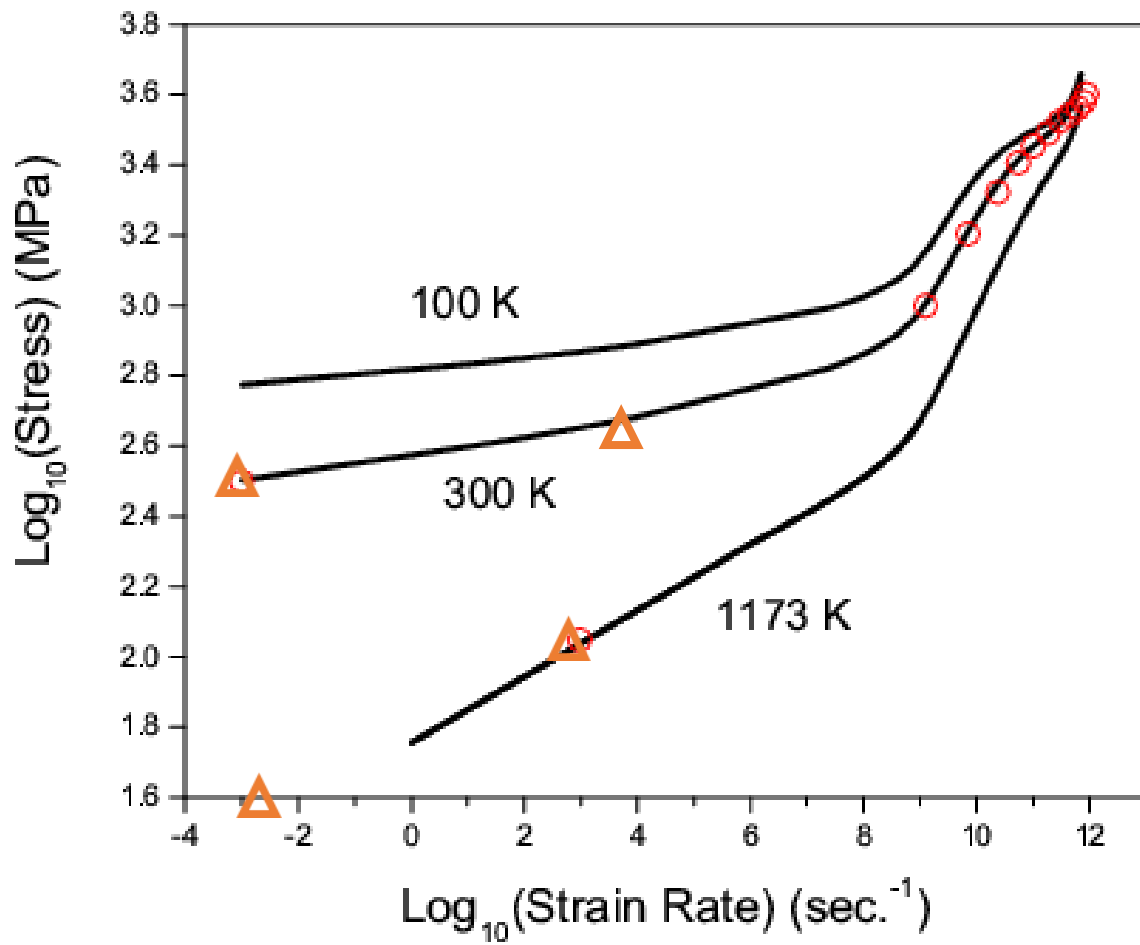
$$q = \tau_0 \dot{\epsilon}^{pl} = b \frac{\tau_0}{\tau(\sigma)} \sqrt{\rho}$$

We already have some important information. For all but very small stresses σ , we can 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 logarithms. The stress is proportional to the Taylor stress, and the proportionality factor is an extremely slowly varying function of its arguments.

The effective temperature analysis tells us that \square is roughly constant in steady state.



Theoretical fits to the PTW data for copper.

Steady-State Parameters

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

Molecular vibration period

$$\chi_0 = 0.25$$

Effective temperature at small strain rates

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

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

$$\mu_{Taylor} = \mu/31$$

$\circ(T)$ = shear modulus $\sim 50 \text{ GPa}$ at 300 K

$$A=2$$

Determines crossover from low to high strain rates.

These are the *only* parameters needed in the steady-state theory for small strain rates.

However, **strain hardening** is a transient phenomenon that involves a few additional rate factors and physical mechanisms.

Equations of Motion

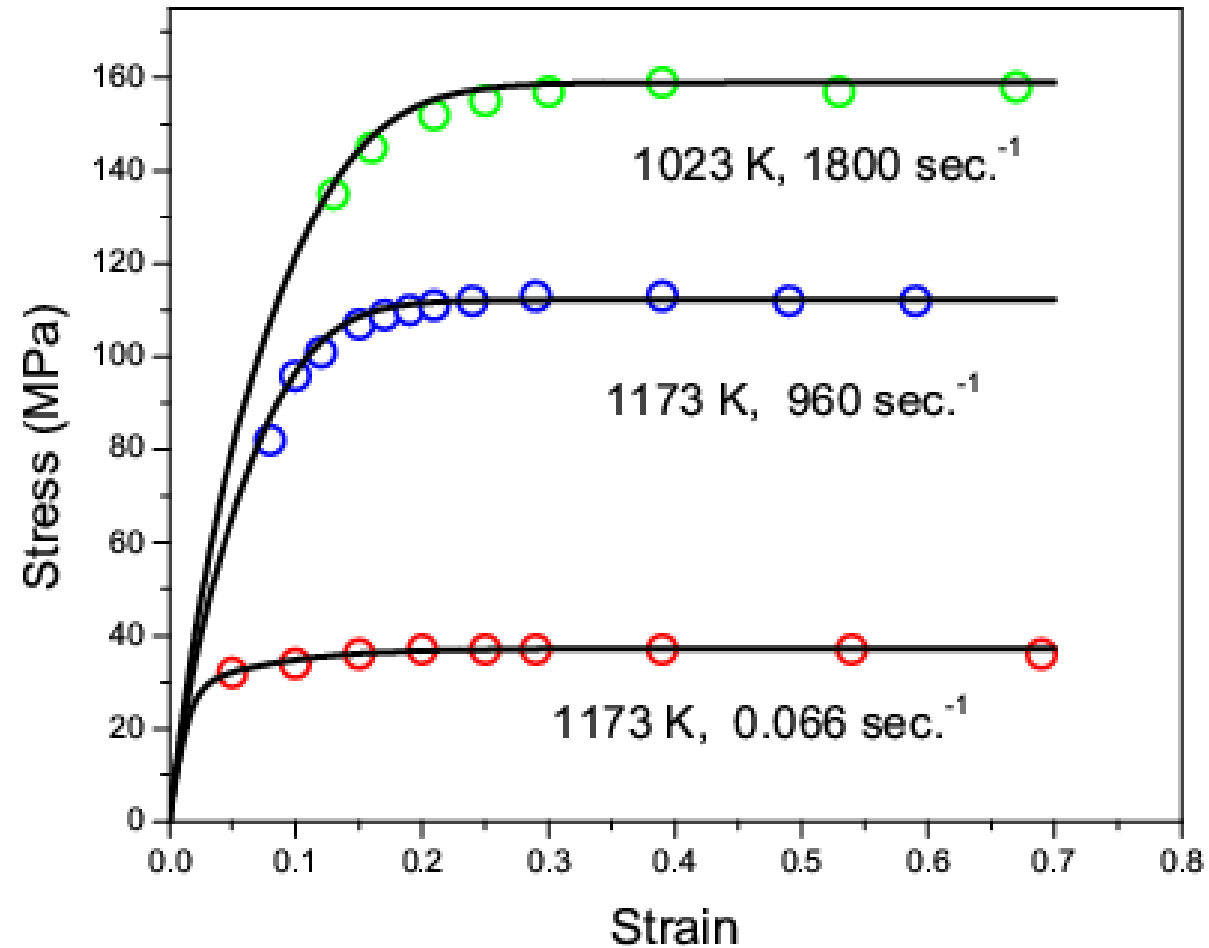
The crucial ingredients are equations of motion for ρ and χ that describe how these quantities approach their steady-state values as functions of time. These equations are:

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

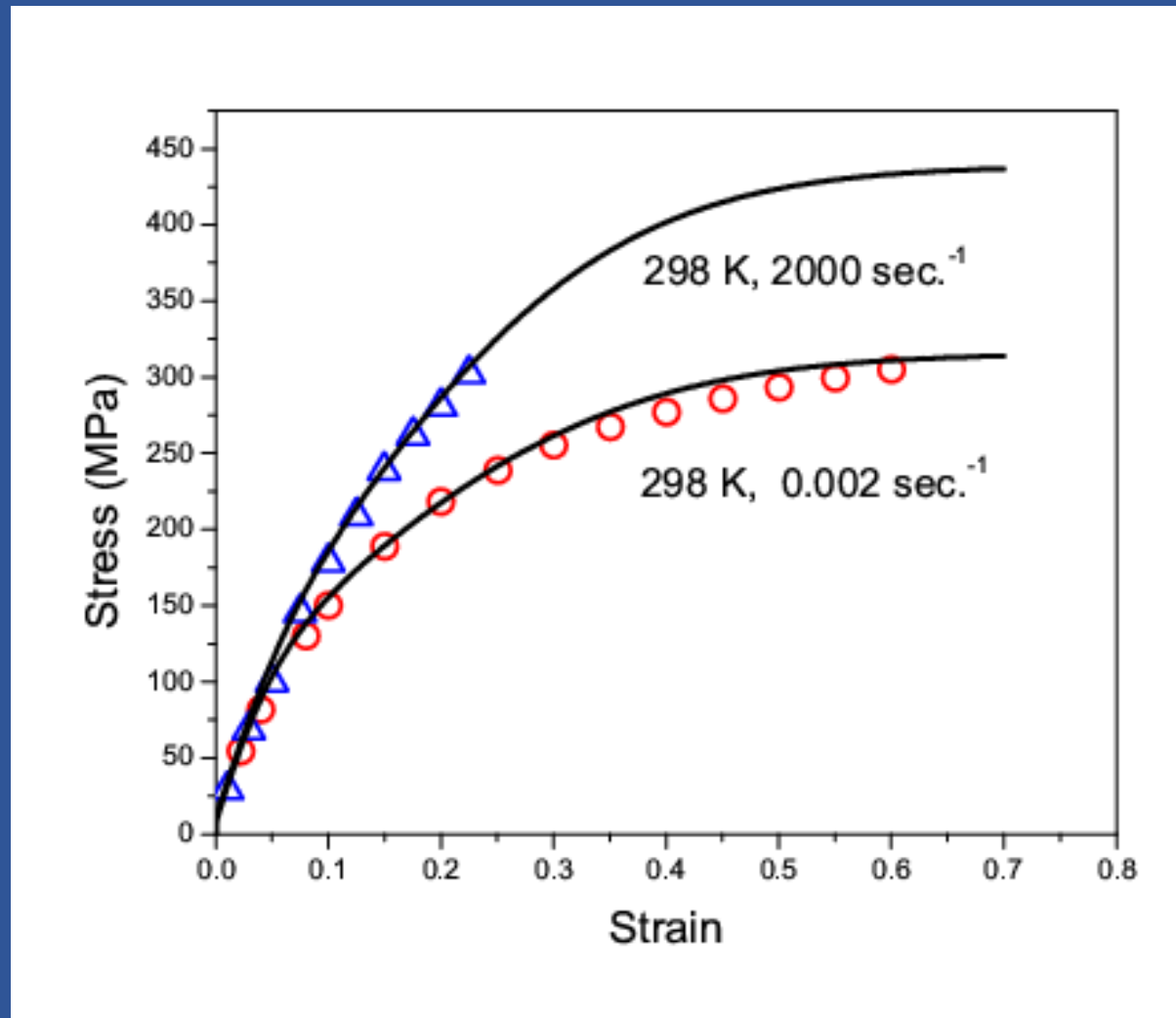
$$c^{eff} \dot{\chi} = \kappa \dot{\epsilon}^{pl} \sigma \left(1 - \frac{\chi}{\chi_0} \right) \quad \text{First law of thermodynamics}$$

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 .

$$\text{Stress equation} \quad \dot{\sigma} = \mu (\dot{\epsilon}^{total} - \dot{\epsilon}^{pl})$$

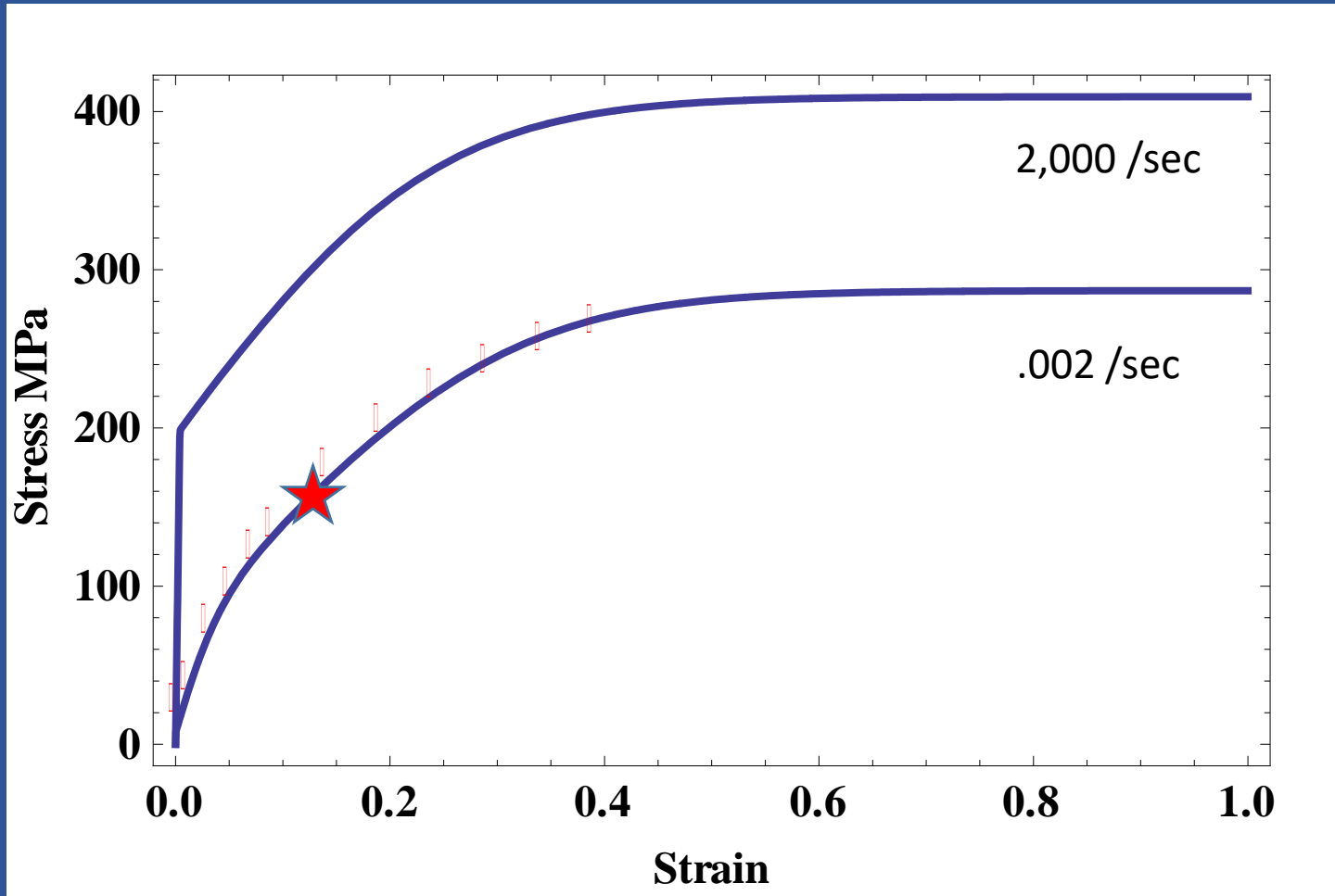


Stress-strain curves for copper at high temperatures, for constant (shear) strain rates as shown. The theoretical curves are from LBL.



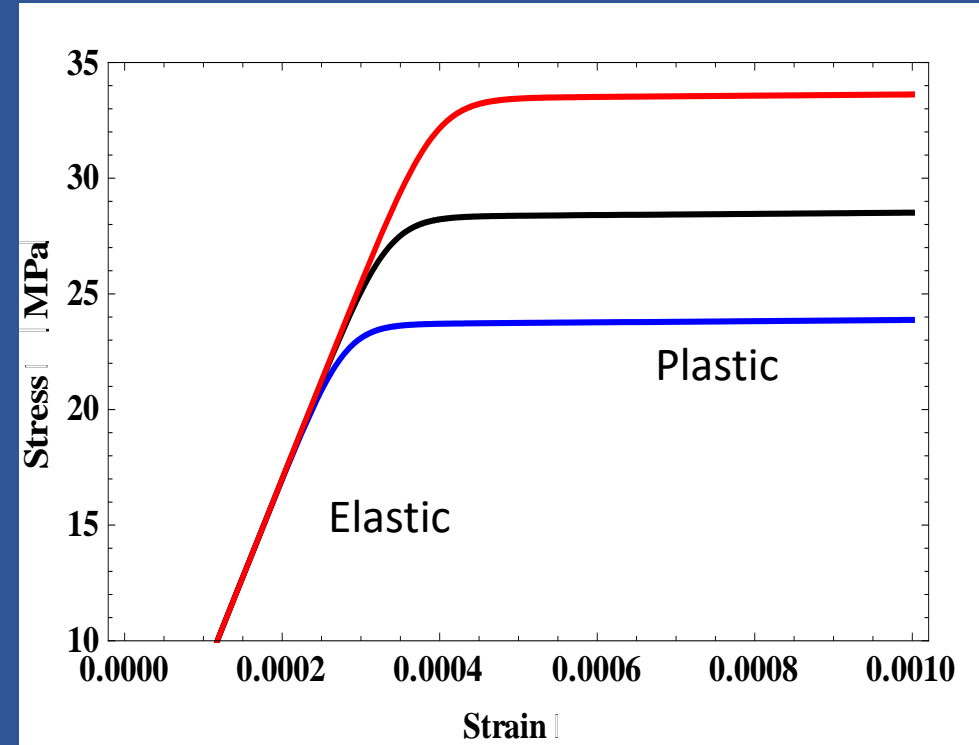
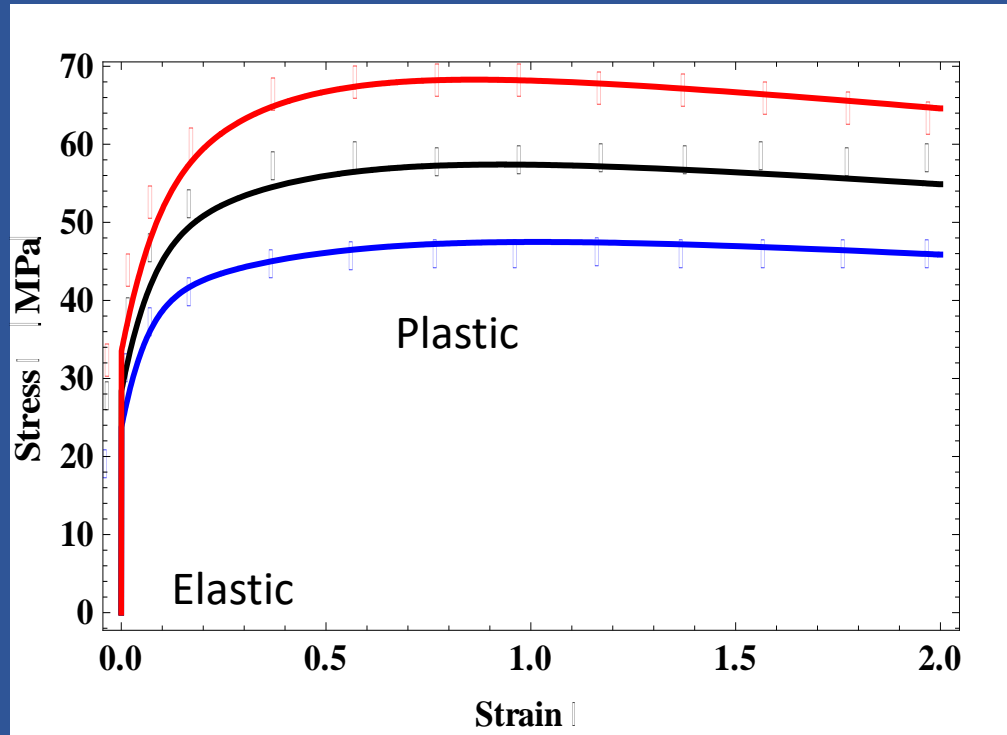
Stress-strain curves for copper at room temperature, for constant, very different, (shear) strain rates as shown. The theoretical curves are from LBL .

Theoretical Experiment



Slowly harden to ★ ; then unload; then reload rapidly. The system remembers its history in the form of increased dislocation density and increased effective temperature (disorder). Note yield stress.

Real experimental data. Shi et al (1997) results for Aluminum at 573 K, at strain rates .25, 2.5 and 25 /sec. Analysis by Le, Tran and JSL (2017)



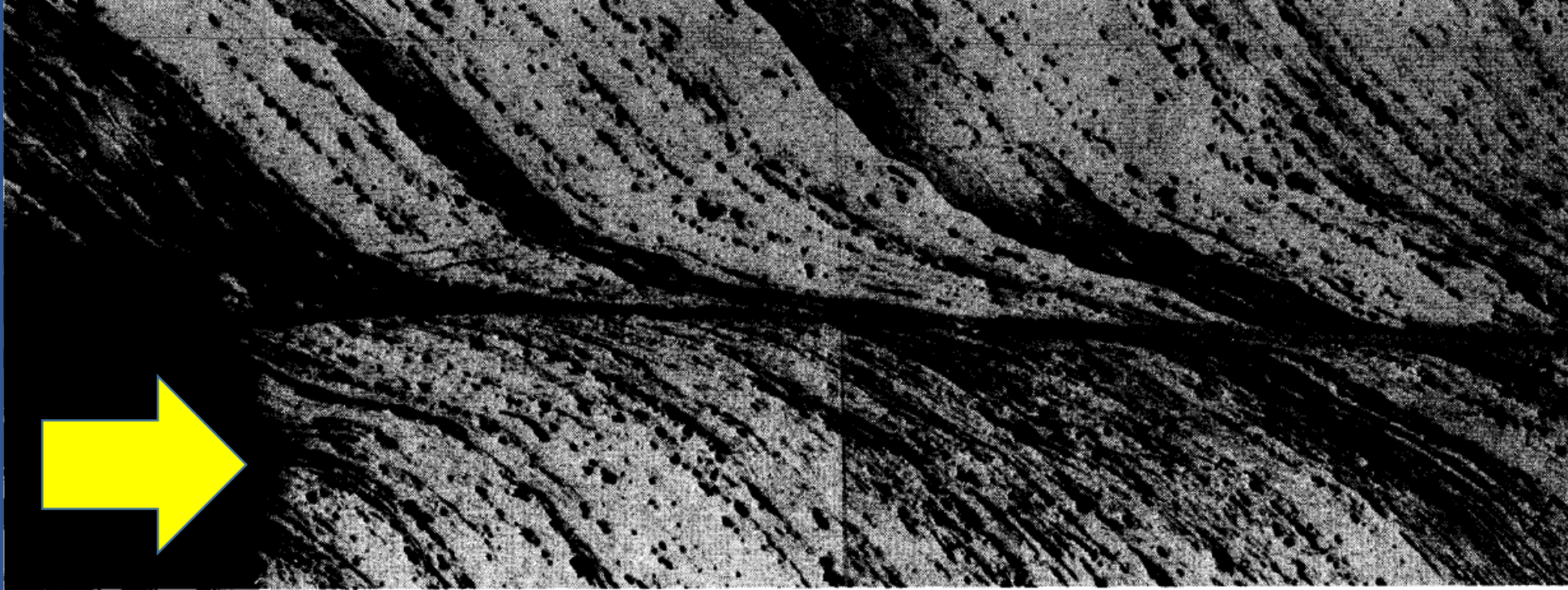
Note sharp yielding transitions – the converse of the almost rate-independent stresses. Also note thermal softening at large strains.

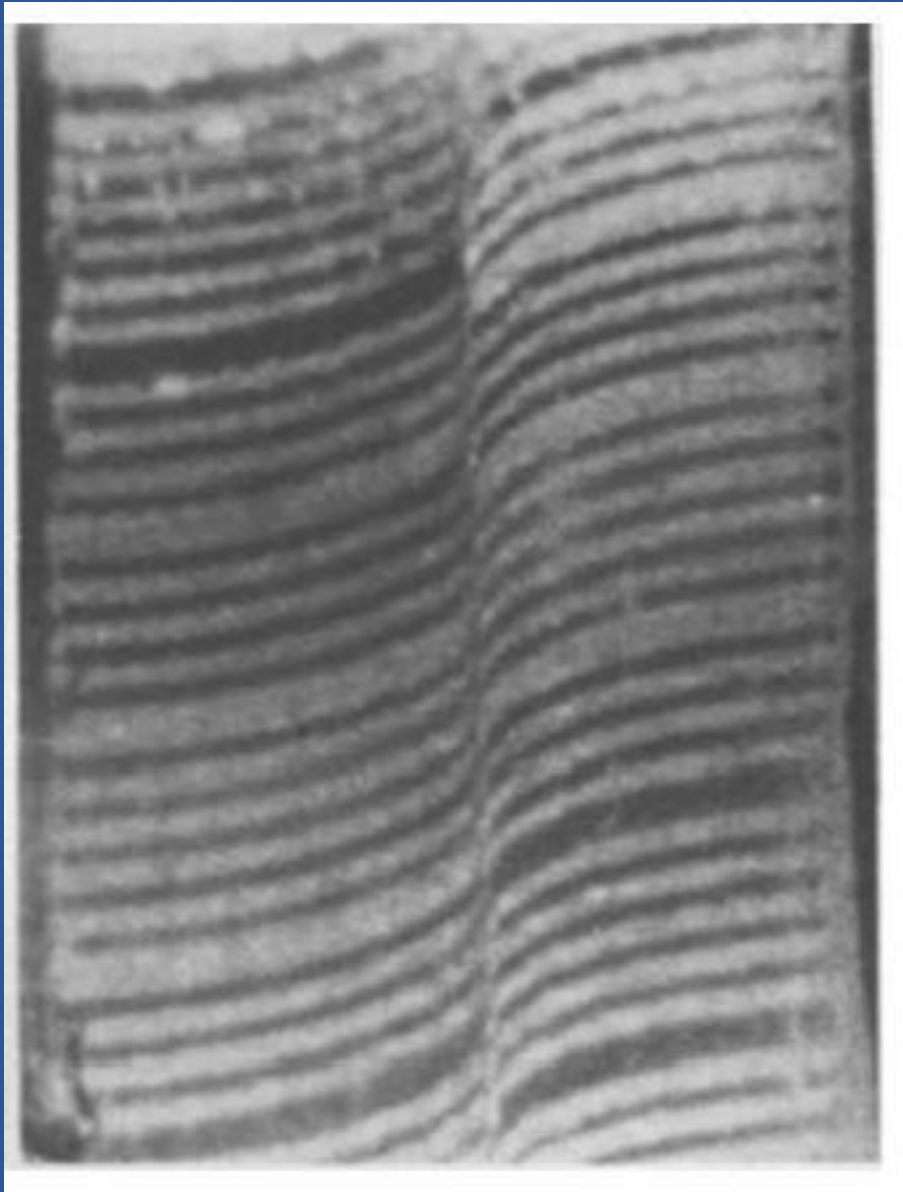
Coupling between thermal and mechanical effects

$$c \frac{\partial T}{\partial t} = \beta \sigma \dot{\epsilon}^{pl} + D \nabla^2 T$$

Ω Is the Taylor-Quinney conversion ratio between input power and heat generation. This coupling is especially dramatic in adiabatic shear banding, which is often a precursor to fracture. “Adiabatic” means that the shearing instability sets in faster than the heat generated is conducted away.

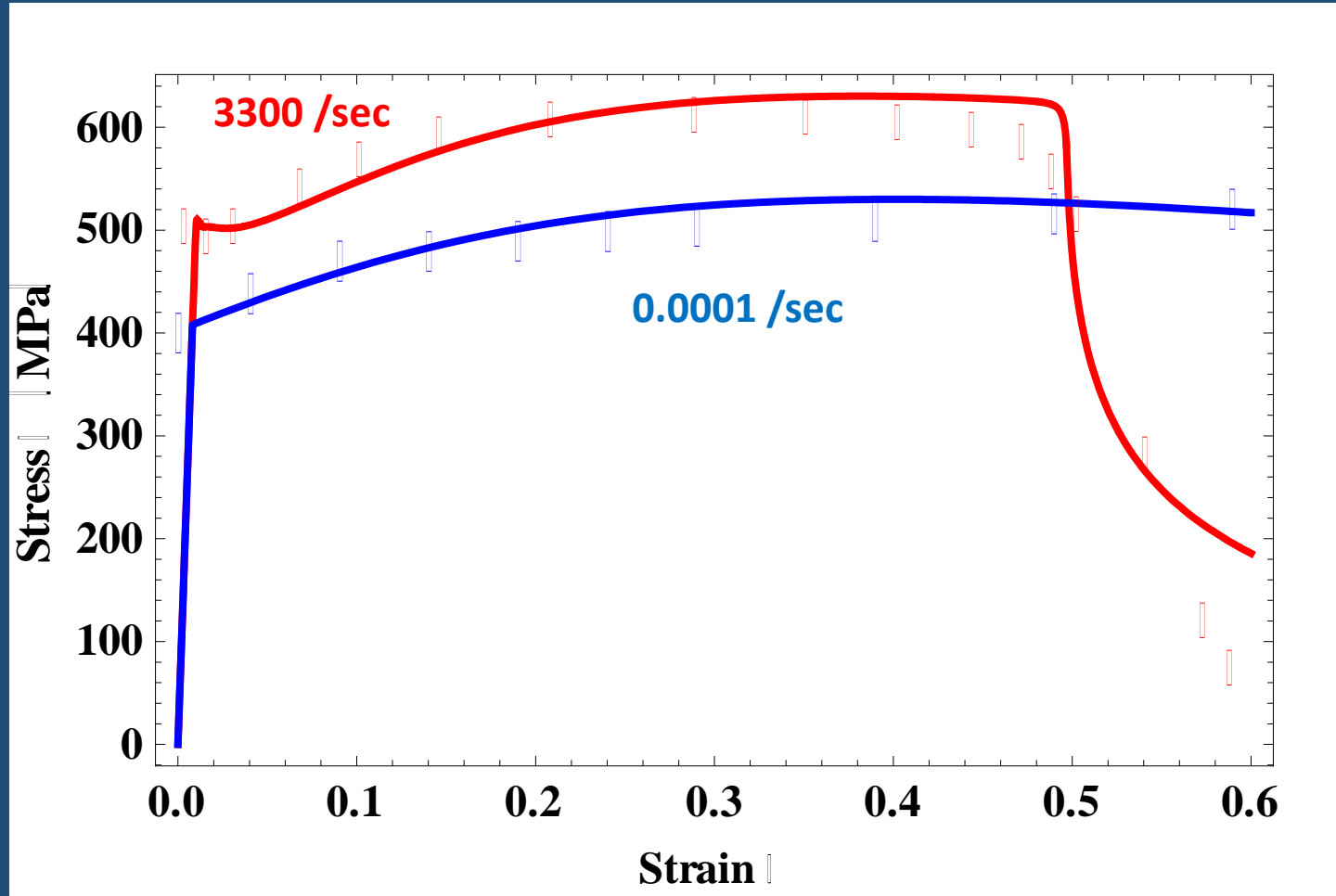
Adiabatic Shear Banding



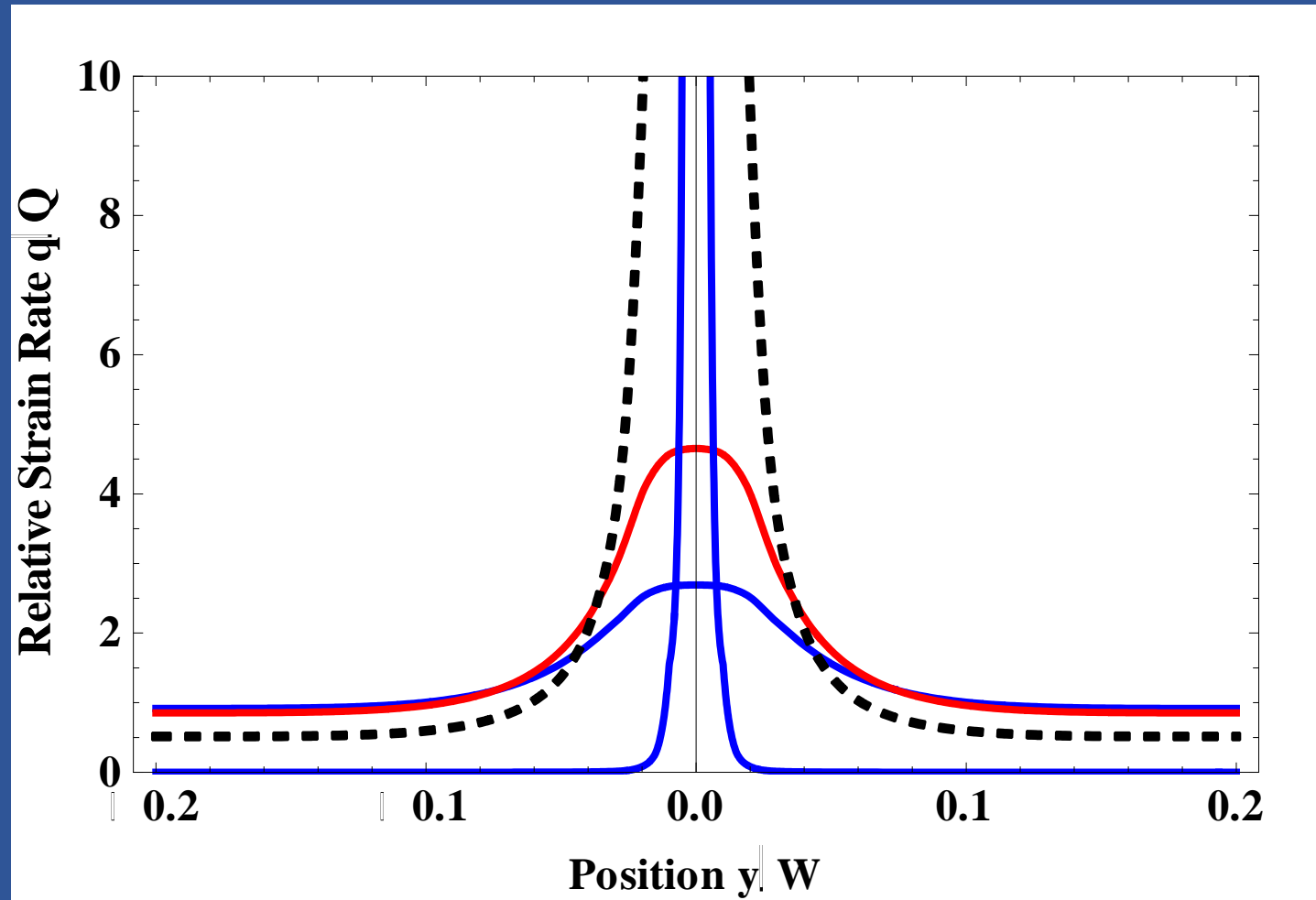


Marchand and Duffy (1988)

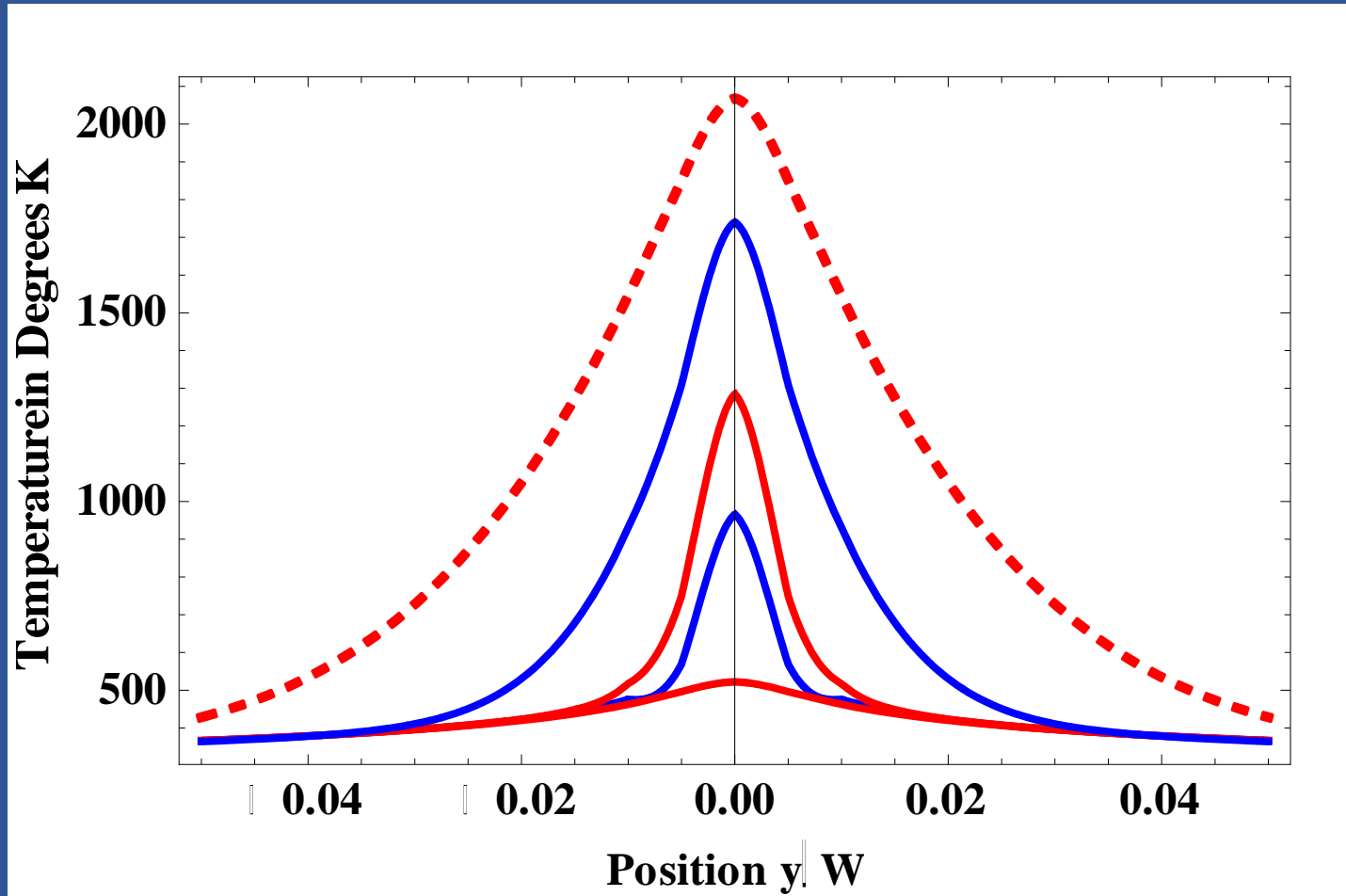
Direct observation of shear deformation near a shear band



Adiabatic shear banding in steel. Data from Marchand and Duffy.
Analysis by Le, Tran and JSL.



Normalized shear rate as a function of position normal to the band. for a sequence of strains during the banding transition. Note that the shear rate collapses to zero outside the band.



Sequence of temperature distributions near the failure point.

JSL PRE 96, 053005 (2017) is a summary of recent progress. In addition to topics covered here, it includes a theory of Hall-Petch grain size effects. (Smaller grains increase the rate of dislocation production in the equation of motion for the dislocation density.)

The next project on the agenda is a theory of fracture toughness and brittle-ductile transitions.