Plastic Deformation in Crystalline Materials

Lecture 1: Overview

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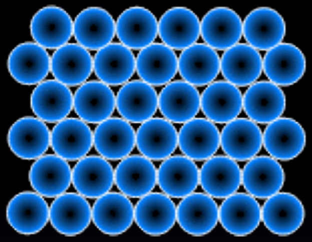
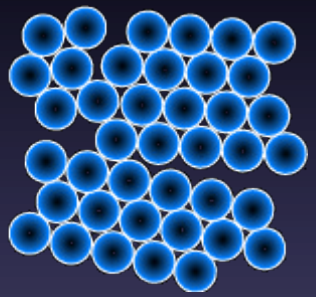
Structure of Solids

Solids:

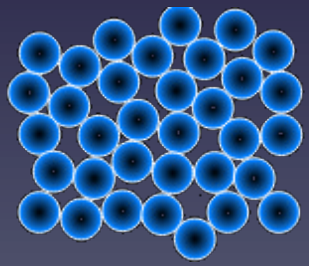
- Crystalline
  - Single Crystalline



  - Poly Crystalline



- amorphous



- Quasi-crystalline* (ordered but not periodic; lacks translational symmetry)

Crystalline vs Amorphous Solids

- Solids are often crystalline.
- A solid may be found in a crystalline or amorphous form. Each may have its own applications
  For example:
- Crystalline silicon (Si) are used in ICs.
- Amorphous silicon (Si) are sometimes used in Li-ion batteries and solar cells
- Amorphous metals are often called metallic glasses
- It is really hard to make some metals amorphous (e.g. Ag)

Let's start with some

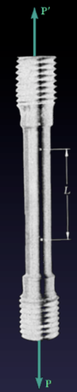
elementary diagrams

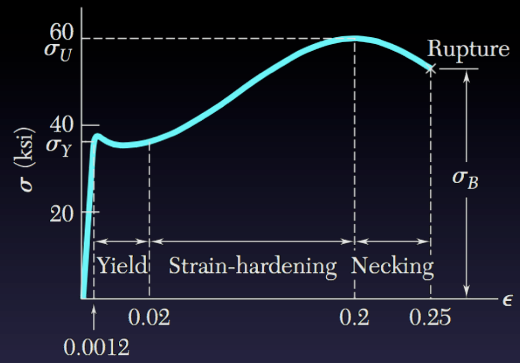
we saw in elementary mechanics of materials and ask

Some questions

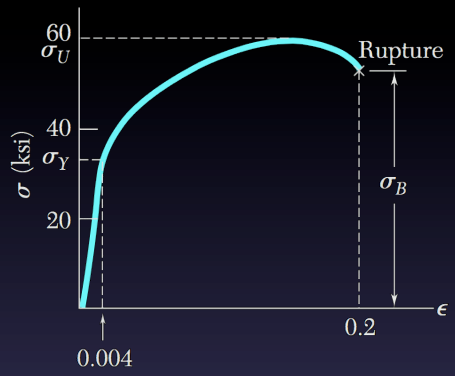
Stress-Strain Curve

Stress-Strain Curve of a metal under uniaxial loading:
One of the first things we learned in mechanics of materials





Low carbon steel



Aluminum Alloy

[Beer & Johnston et al, mechanics of materials]

Questions:

- Why do materials become plastic? What is the mechanism of plastic deformation?
- Why stress-strain curves of different materials are different?
- How can we model strain hardening (= work hardening)?

Stress-Strain Curve – Loading and Unloading

Again what we saw in the first chapters of mechanics of materials

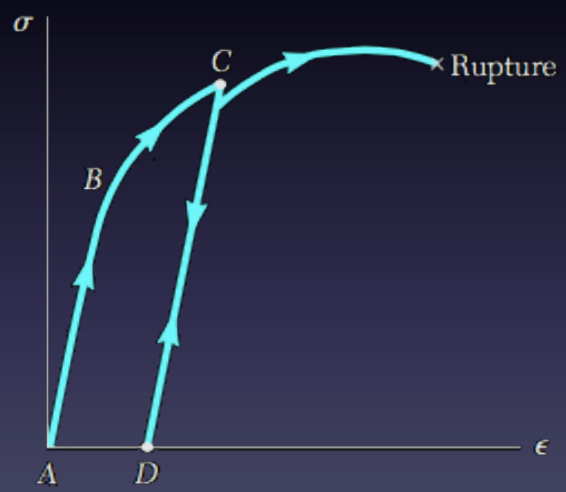


Fig. 2.14 Stress-strain characteristics of ductile material reloaded after prior yielding.

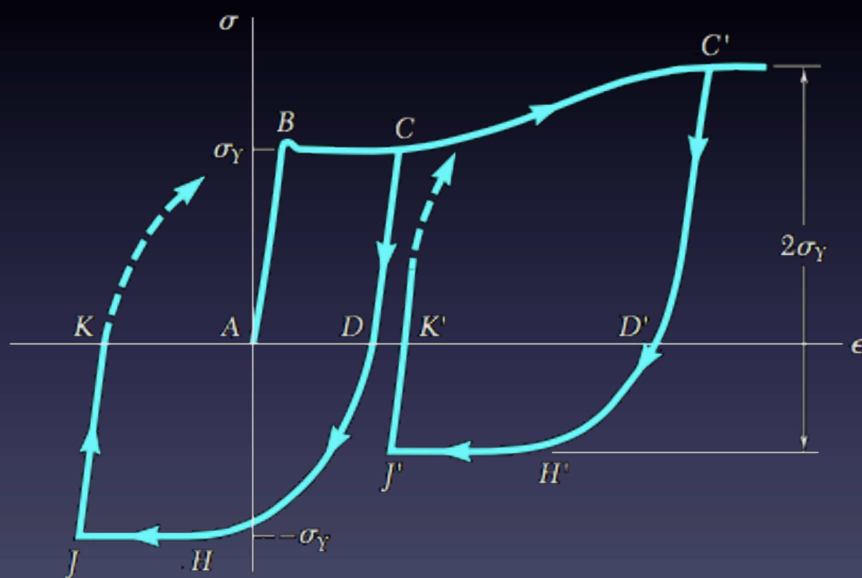
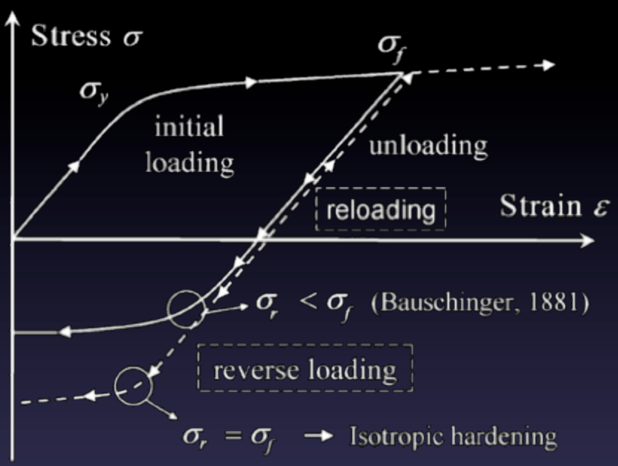


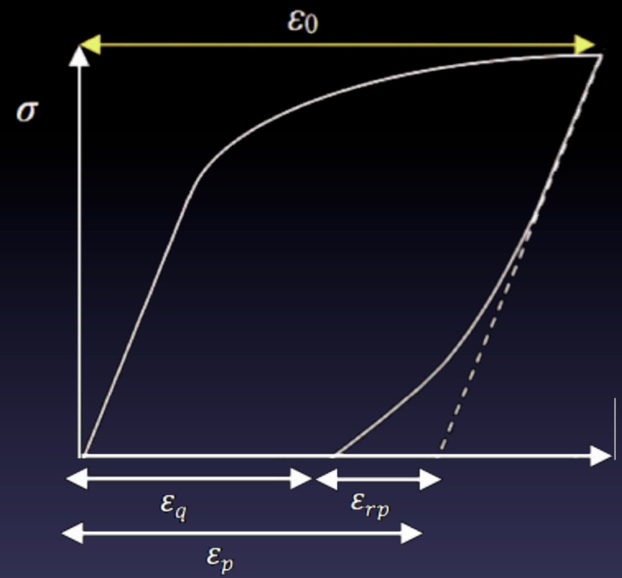
Fig. 2.15 Stress-strain characteristics for mild steel subjected to reverse loading.

[Beer & Johnston et al, mechanics of materials]

Bauschinger Effect



[Xiang, Vlassak, Acta Mater, 2006]

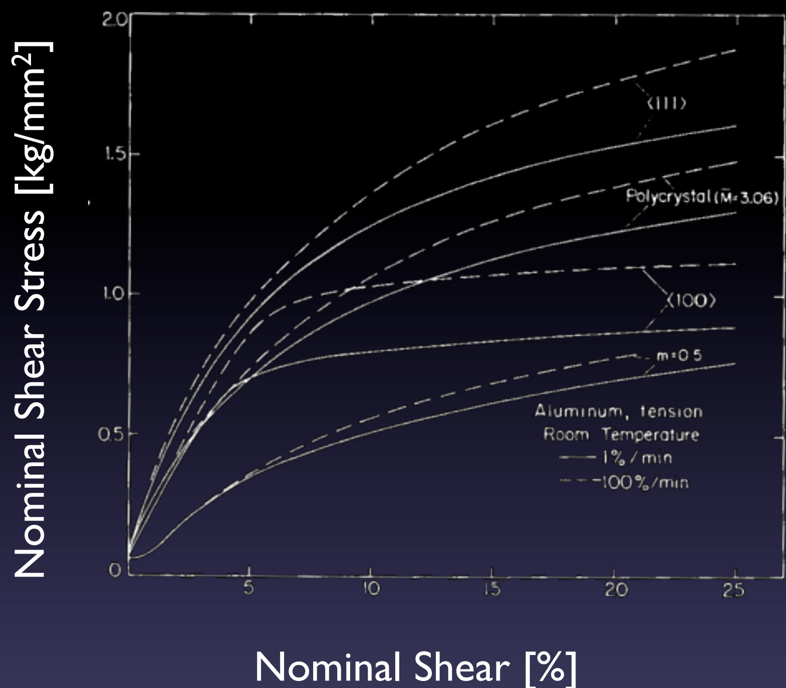


ε_0: total strain
ε_p: plastic strain or hypothetical residual strain
ε_q: residual strain
$\varepsilon_{rp} = \varepsilon_p - \varepsilon_q$: reverse plastic strain

Question:

What causes the Bauschinger effect?

Effects of Orientation & Loading Rates



Nominal stress strain curves (without correction for area changes and orientation changes) for 99.99% pure Al, at two tensile strain rates: three single crsytals of different orientations and one polycrystal of a grain size of 0.2 mm. After Kocks et al., Work Hardening, 1968

Questions:

- How does the orientation affect the deformation?
- What is the difference between deformation of single crystal and polycrystal?
- How does the loading rate affect the deformation?

Effects of Temperature

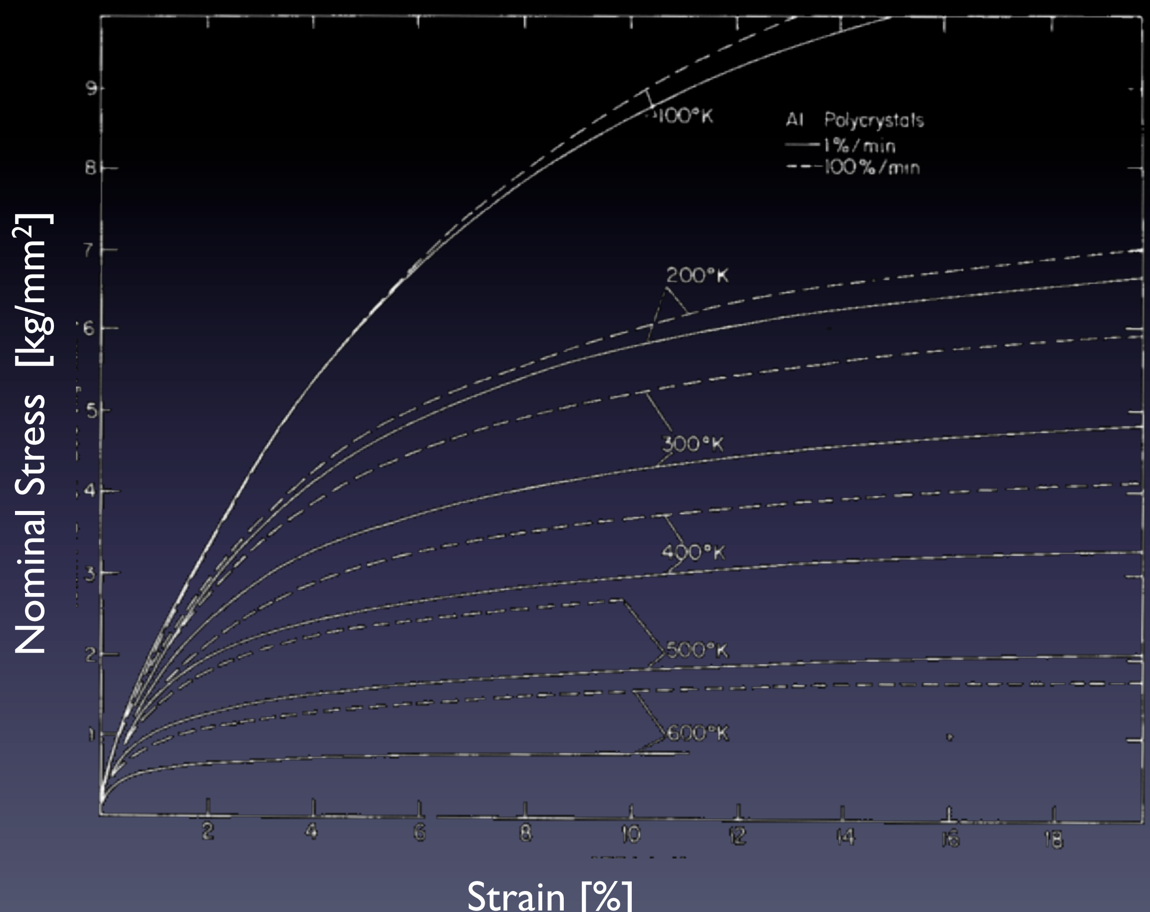
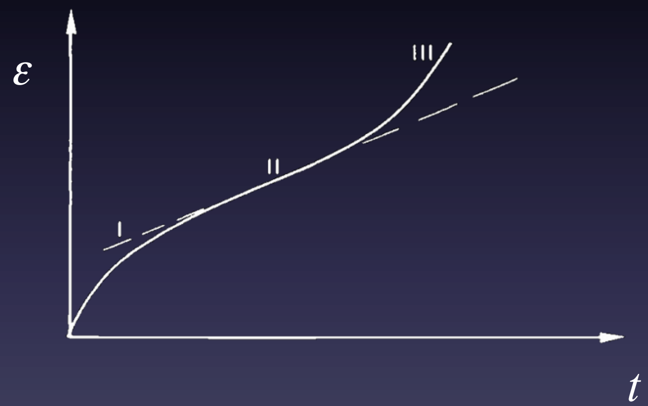


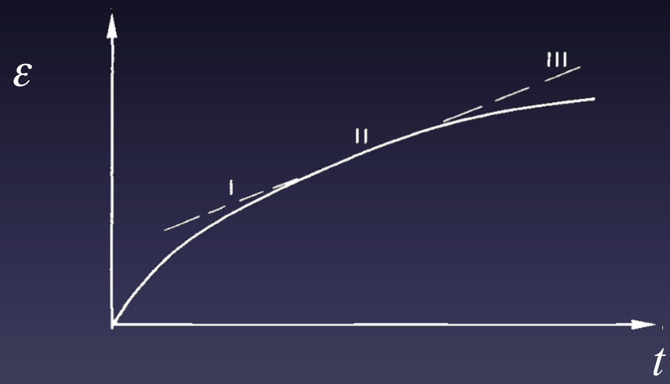
Fig. 19—Tensile stress-strain curves, at two tensile strain rates and at various temperatures, of 99.99 pct Al polycrystals of a grain size of 0.2 mm (15 pct of the grains being on the surface). After Kocks *et al.*[72]

Question:
How does the temperature affect the hardening rate?

Creep



strain vs time (in tension)

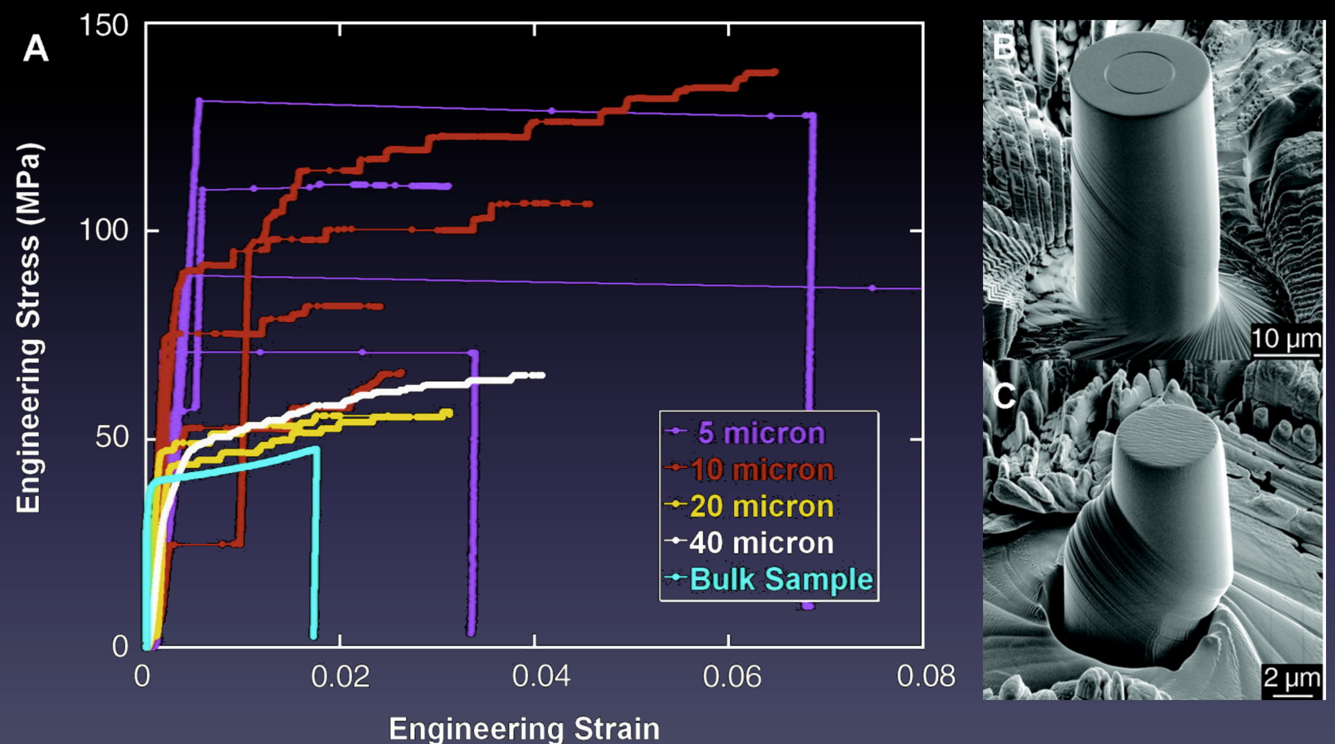


strain vs time (in compression)

Three stages: (I) primary creep regime (II) quasi-steady-state regime (III) tertiary creep regime

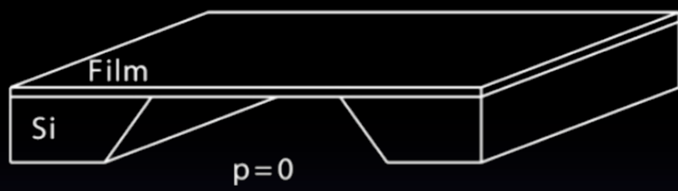
Question: What is the explanation for each regime?

Size Dependent Behavior: Experiment

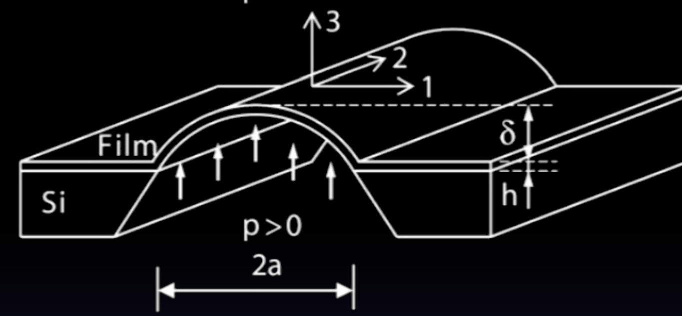


Pure Ni microsamples having a <134> orientation (A) stress-strain curves for samples with different diameters (B) SEM image at 4% strain (diameter 20 μm) (C) SEM image at 19% strain (diameter 5 μm) [Uchic et al., Science, 2008]

Another Experiment: Bulge Test



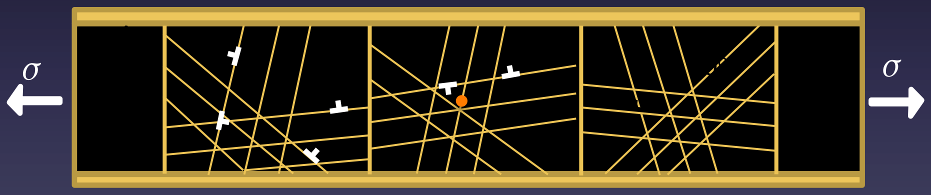
before pressure is applied



after pressure is applied

[Xiang, Vlassak, Scripta Mater., 2005]

Plane Strain Model:

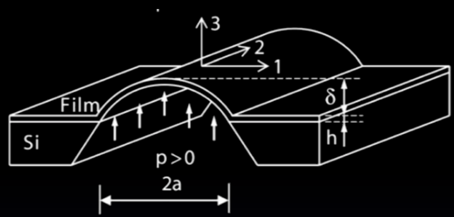


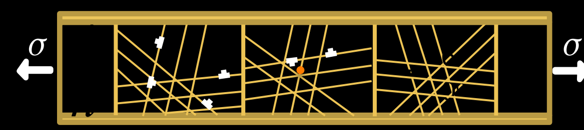
- Applied pressure p and membrane deflection h are measured
- Average stress and strain are determined using following (or more sophisticated) expressions

$$\sigma = \frac{pa^2}{2h\delta}, \qquad \varepsilon = \varepsilon_0 + \frac{2\delta^2}{3a^2}$$

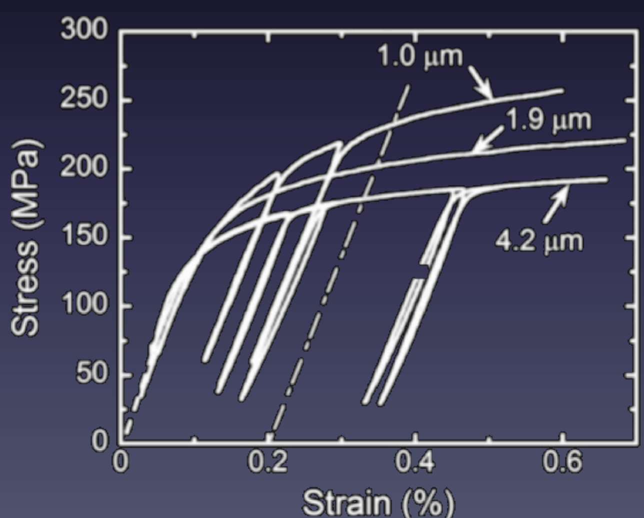
ε_0 : residual strain in the film

Bulge Test - II



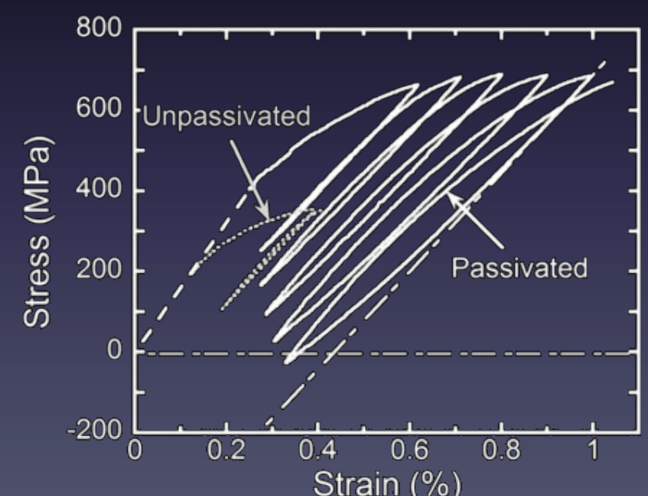


Effect of Film Thickness:



Cu Films with both surfaces passivated of different film thicknesses

Effect of Passivation:

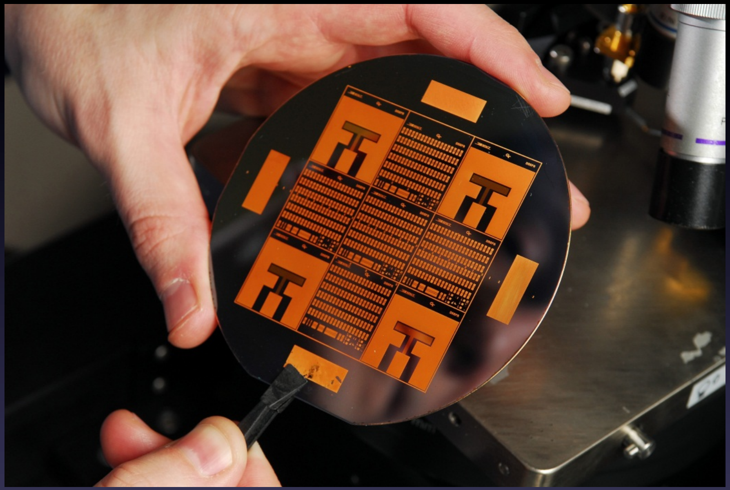


Cu film of thickness h = 340 nm

[Xiang, Vlassak, Acta Mater., 2006]

Importance of Study of Mechanical Behavior of Materials at Small Scales

Detailed and quantitative understanding of size effect is essential for a reliable design



http://gtresearchnews.gatech.edu/newsrelease/mems-cad.htm

Many of failure mechanisms are stress-driven

It is critical to know the strength of a component in a device and hence the level of stress it can support

Size Effect

1924 — First Report by G.I. Taylor

1950s — Hall – Petch effect
Brenner’s paper on whiskers
Conference in NY

1980s — Small Scale Devices

1990s — Experiments exhibited size dependence

Continuum Mechanics Approach for Size Effect

In classical approach:

$$\dot{\sigma} = function(\dot{\varepsilon}, T, \ldots)$$

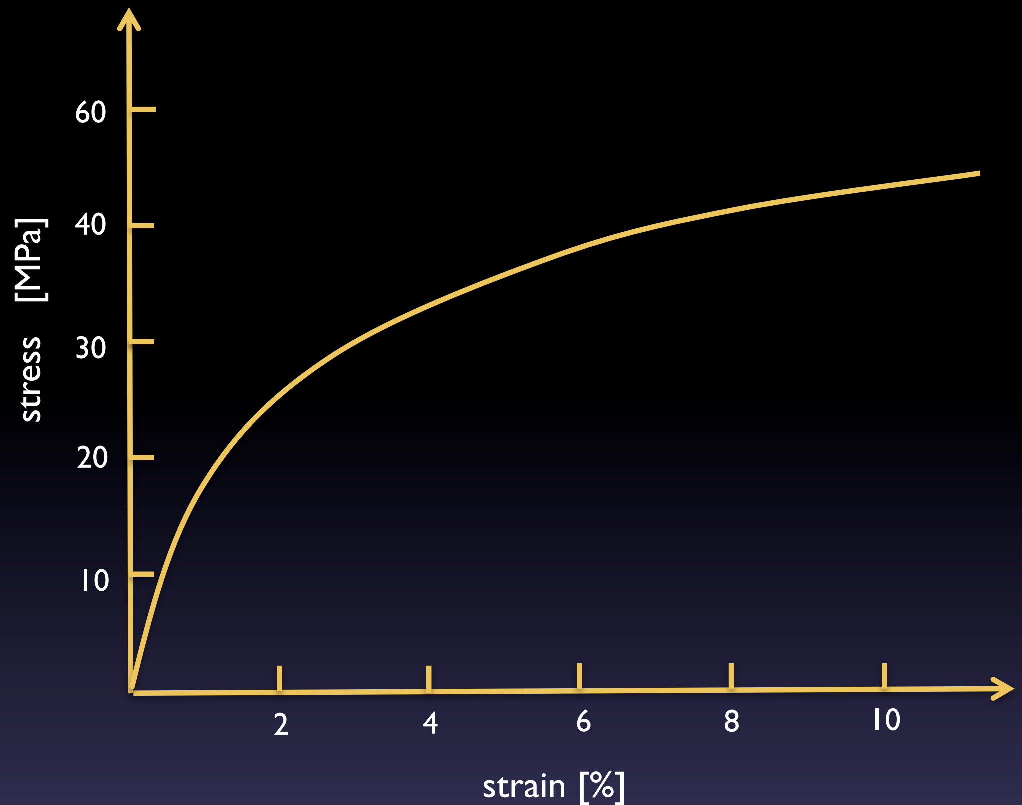
$$f(\sigma_{ij}, \varepsilon_{ij}^{p}, k) = F(\sigma_{ij}, \varepsilon_{ij}^{p}) - k^2(\varepsilon_{p}^{e}) = 0$$

In nonlocal approach

$$\dot{\sigma} = function(\dot{\varepsilon}, \nabla\dot{\varepsilon}, \nabla^2\dot{\varepsilon}, \ldots, T, \ldots)$$

This requires introduction of one or more length parameters into the constitutive equation

There is no strain gradient theory that can be applied to all experiments



(Kocks, Trans ASME, 1970)

"it is sometimes said that the turbulent flow of fluids is the most difficult remaining problem in classical physics. Not so. Work hardening is worse." (A.H. Cottrell, 2002)

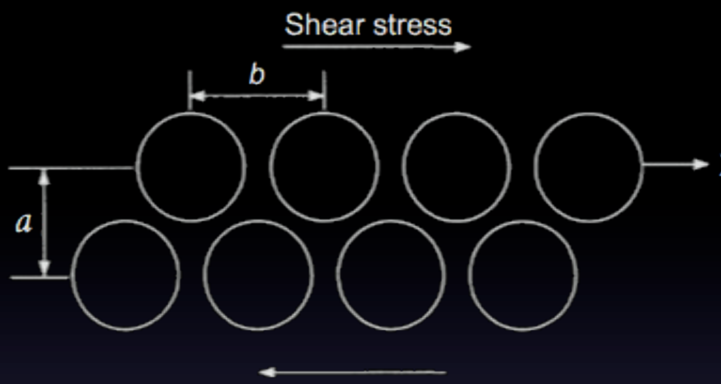
One Solution

- We should consider why and how crystals deform plastically.

Ideal Shear Strength

Consider a single crystal

$$\tau = \tau_{\max} \sin \frac{2\pi x}{b}$$



If $\tau < \tau_{max}$: shear strain is elastic and will disappear when the stress is released.

For very low value of $\gamma = x / a$: $\tau = G\,\gamma$

Therefore:

$$\left(\frac{d\tau}{d\gamma}\right)_{x\to 0} = G$$

$$\tau_{\max} = \frac{Gb}{2\pi a} \approx \frac{G}{2\pi}$$

More accurate calculations showed that τ_{max}= G/30 which is still >>measured shear strength

Why materials become plastic

Ideal shear strength >> measured shear strength

81 years ago : Dislocations



G.I. Taylor   Egon Orowan   Michael Polyani

Work hardening was the first problem that was considered

16 volumes of "Dislocations in Solids"

1953 A.H. Cottrell: [Work hardening] was the first problem to be attempted by dislocation theory and may be the last to be solved

2003 U.F. Kocks & H. Mecking Work hardening is as hopeless as ever

2009 L. Kubin: There is presently no generally accepted theory explaining how and why organized dislocation microstructures emerge during plastic flow

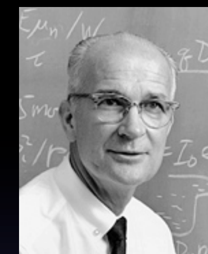
Work hardening was the first problem that was considered

G.I. Taylor

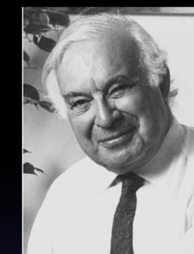
Egon Orowan

Nevil Mott*

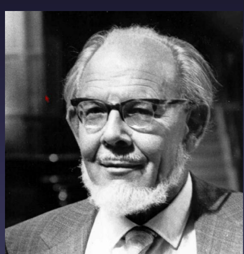
Rudolf Peierls*



William Schockley*



F. Nabarro

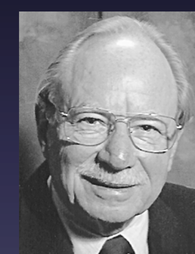


Frederick C Frank

Alan Cottrell

J. Friedel

T Mura



U Fred Kocks

H. Mecking

John Hirth

Jens Lothe

J. & J. Weertman

Ladislas Kubin

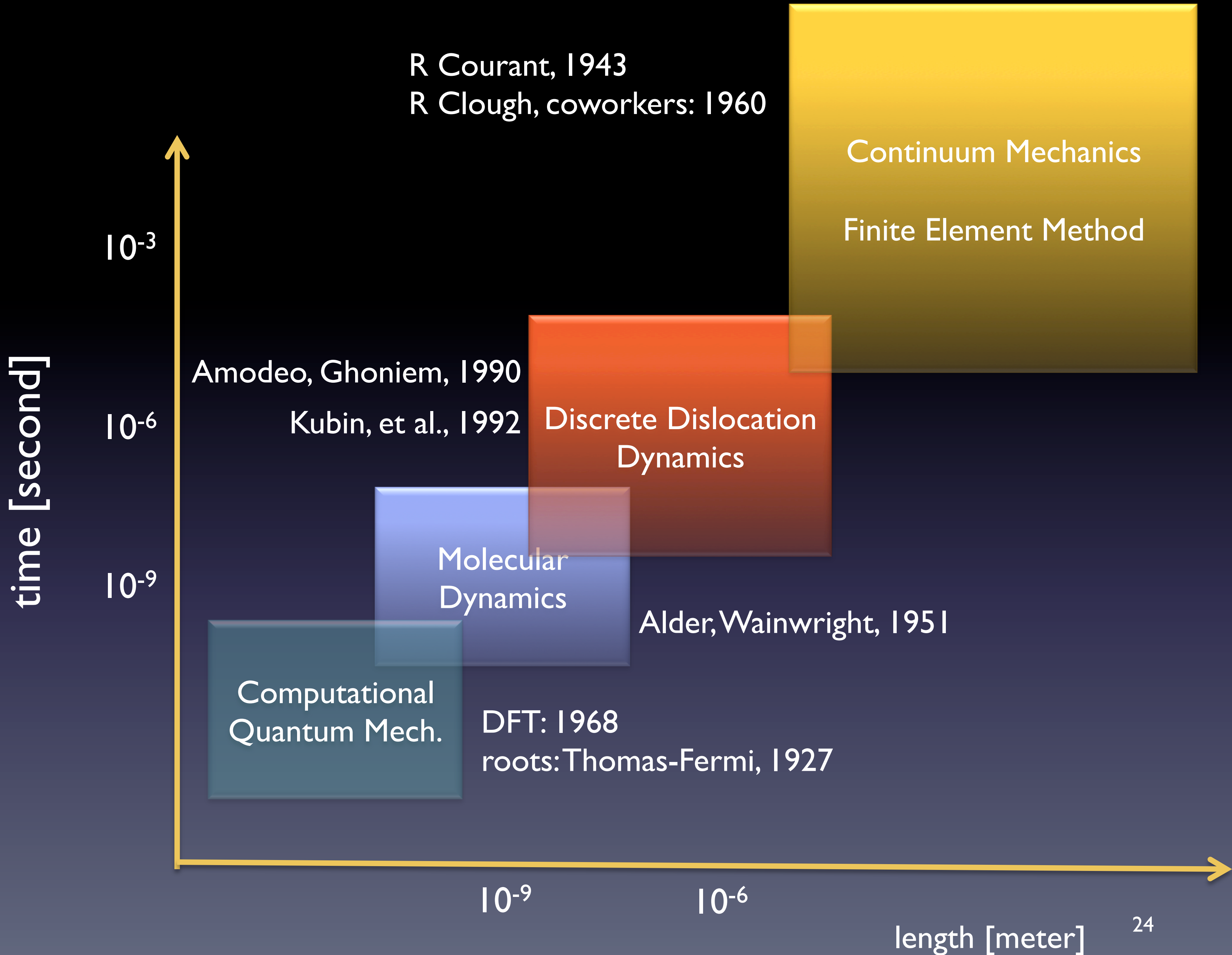
* Nobel Laurites

Work Hardening Modeling

- Collective motion of dislocations → Plastic Deformation

- Individual processes are well understood
- Understanding overall effects is challenging without computer modeling

some main processes into the model
→ Discrete Dislocation Dynamics


R Courant, 1943
R Clough, coworkers: 1960
Continuum Mechanics
Finite Element Method
10-3
time [second]
Amodeo, Ghoniem, 1990
10-6
Kubin, et al., 1992
Discrete Dislocation Dynamics
10-9
Molecular Dynamics
Alder, Wainwright, 1951
Computational Quantum Mech.
DFT: 1968
roots: Thomas-Fermi, 1927
10-9
10-6
length [meter]