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Bridging Length Scales

#11: Real crystals

From earlier study of perfect crystals:

•Yielding occurs by crystal slip. The slip vector is a lattice translation vector so that the crystal structure is preserved when the crystal deforms not matter how large the plastic strain.

•The "ideal" yield stress is given by $\sigma_{ideal} = \frac{b}{d}$ where b is the slip vector which lies in the slip plane, and d is the distance between the slip planes.

•The largest value of d is obtained for the planes which have the highest packing of atoms in it.

•The smallest value of b must occur in the plane with the highest packing, which is the same as the planes with the highest value of d.

The study of "perfect" crystals

•The lowest value of σ_{ideal} occurs on specific slip systems in a crystal. For example the slip vectors in the family <110> and slip planes in the family {111} - for the fcc system (they can usually be identified by inspection). Each combination of slip vector and slip plane must be such that these slip vector and the plane vector are perpendicular to one another. In this way various combinations for the slip systems in the same family can be obtained.

•In fcc there are 12 such "independent" slip system. The same in the bcc crystal.

•The yield stress of bcc crystals is always somewhat higher than for fcc crystal because the lengh of the slip vector is higher in the bcc structure.

Concepts for "real" crystals

It is rather interesting that the predictions for ideal crystals serve as good guidelines for plastic deformation in real crystals even though real crystal have a much, much lower yield stress. They deform by "line defects", called dislocations, for example,

•the result that the slip systems with the lowest yield stress will also have the lowest value of $\frac{b}{d}$.

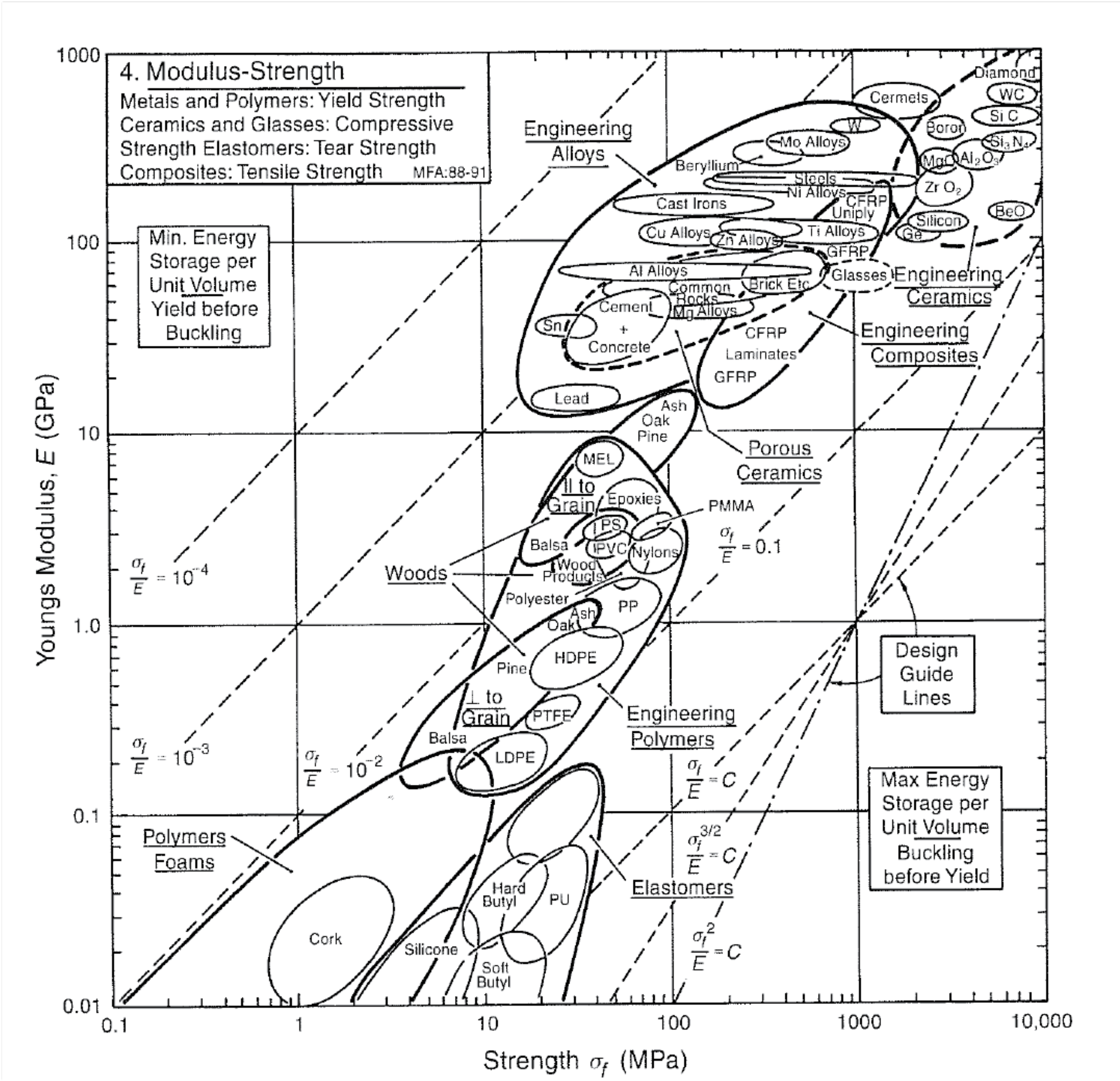
•the ideal yield stress was derived to be approximately given by $\sigma_{ideal} = 0.2G$, that is the yield stress was proportional to the shear modulus. Recall that:

$$G = \frac{E}{2(1+\nu)}$$

Therefore assuming that the Poisson's ratio do not change much (they usually lie in the 0.2-0.33 range), which will give $[\sigma_S]_{ideal} \rightarrow [\sigma_Y]_{ideal} \approx 0.1E$, that is the tensile yield stress is about 10% of the Young's modulus. Here σ_Y is the yield stress in uniaxial tension

The yield stress of real crystals, even though much lower than that of ideal crystals, still scales with the elastic modulus.

The realistic value of the yield stress of real metals, even when engineered to a high degree (for example tool steels) rarely exceeds 0.01E, that is, they reach their elastic limit at 1% strain.



What controls the yield stress of real crystals?

Real crystals contain defects, they are called dislocations. They have the following properties:

•They are "line" defects, that is, they meander through the crystal like a line. The vector of this line is one of the basic property of dislocations

•A dislocation has a specific slip vector, also equal to $\vec{b}$, as in σ_{ideal}. The slip vector remains the same no matter what the direction of the line vector. The dislocations move in slip plane as defined by the slip system in the ideal crystal. **Therefore the dislocations move as in the case of the "ideal" crystal.**

• The yield stress is now given by the shear stress which must be applied to the crystal so that the dislocation line can cut through the entire slip plane in a crystal.

Dependence of the yield stress of single crystals and polycrystals of engineering materials (i.e. with dislocations).

•Yield stress of pure single crystals (but with dislocations)

•Yield stress controlled by barriers to dislocation motion

(i) Grain boundaries; polycrystals have a higher yield stress than single crystals

(ii) Hard particles that pin the dislocations.

Yiela Stress of Single Crystals measured at 300K at a strain rate of 1e-04 per sec

(Recall that that the ideal yield stress is expected to be 0.1*E, or 0.25*G

Crystal Class	Metal	Yield stress in MPa	Actual Yield Stress/G
FCC	Al	0.5	2.00E-05
	Cu	0.5	1.20E-05
	Au	0.5	2.00E-05
	Ni	2	2.50E-05
	Ag	0.4	1.50E-05
	NaCl	1	6.60E-04
BCC	Fe	15	1.80E-04
	Nb	20	5.20E-04
	Mo	70	5.60E-04
HCP	Cd	0.13	5.00E-05
	Mg	0.5	2.80E-05
	Zn	0.3	8.00E-06

Notes:

•Actual yield stress is commonly three to four orders of magnitude lower than the ideal yield stress

•BCC crystals have a ten times or more higher yield stress than FCC crystals (why?)

•Zinc polycrystals are brittle even though single crystals are soft and malleable (only three slip systems). However, FCC crystals are also malleable but not brittle.

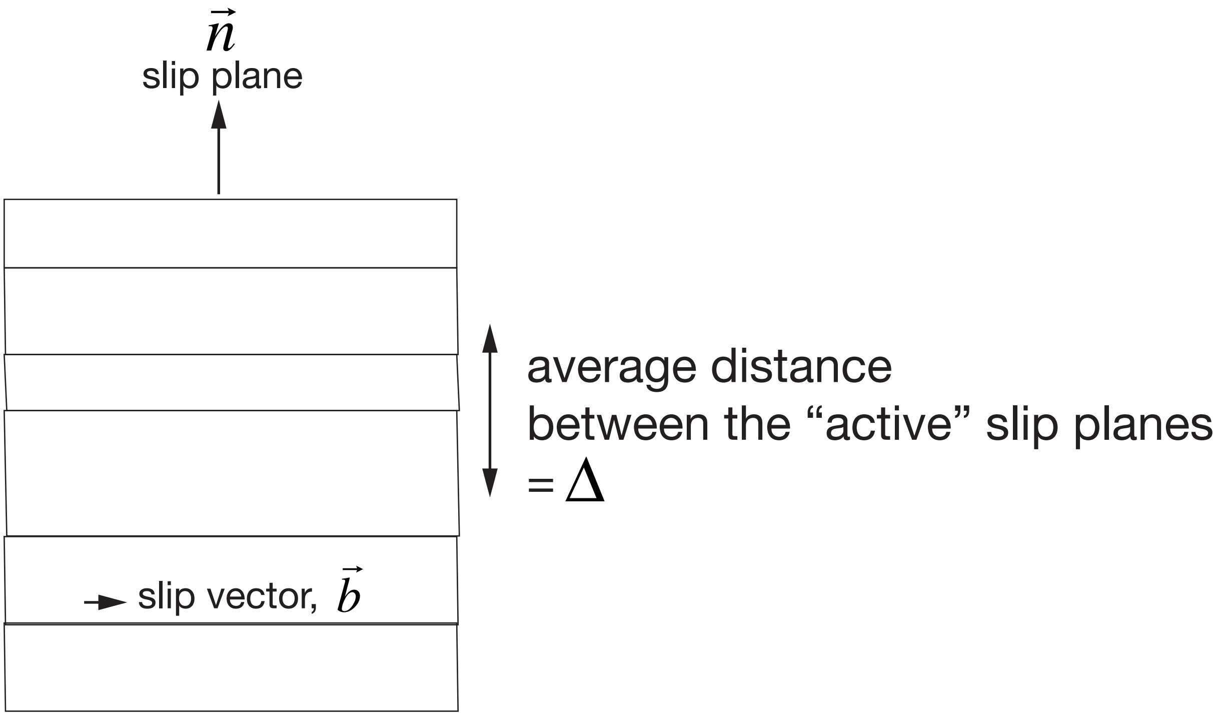
Description of slip in a single crystal

•significance of the distance between the active slip planes

•significance of the number of slip steps in a given slip plane

•relationship of the plastic strain to the above parameters.

•The definition and the significance of the dislocation density. Average spacing between the dislocations. How that relates to the plastic strain.

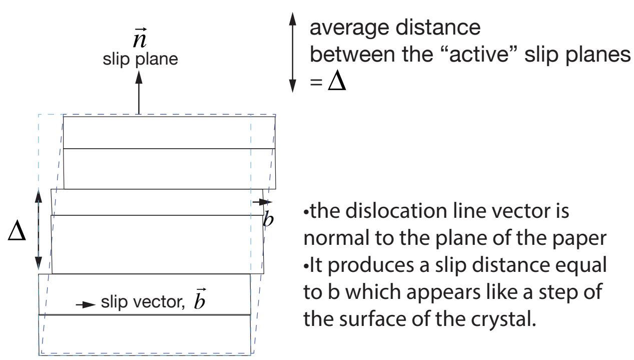


Notes:

•the spacing between activated slip planes, Δ, is several micrometers (10 -100 μm) - can be see with an optical microscope.

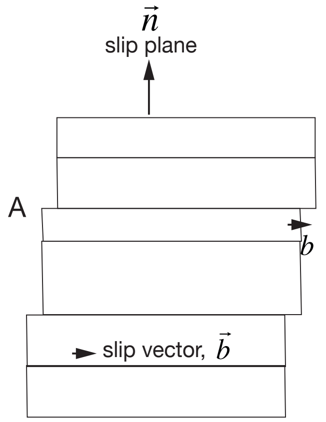
•In a single crystal the glide of dislocation (sliding of a dislocation) fully across the slip plane leads to slip step on the surface of the crystal equal to $\vec{b}$.

Description of slip in a polycrystal crystal



Question: how much plastic stain when slip occurs as above:

$$\gamma_P = \frac{b}{\Delta}$$



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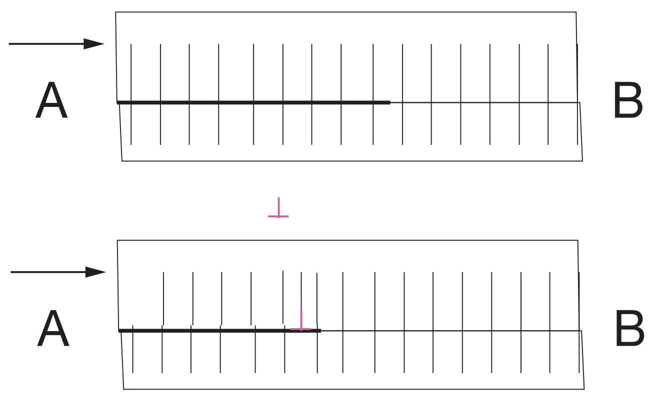
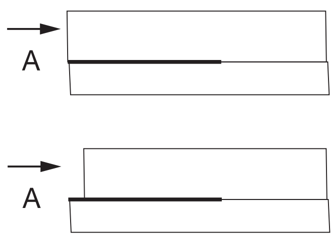


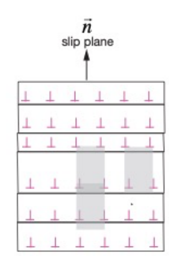


the displacement has to be a slip vector since the crystal structure is conserved.

•In the above example the dislocation (pink) is a line normal to plane of the paper, AND, it has a slip vector equal to “b” . This one dislocation sliding (gliding) through the entire slip plane across the crystal will produce step equal to b.

Plastic strain from many dislocations?

We consider cells of dislocations as shown on the right. The distance L is both the distance between the dislocations and the distance between the glide planes. If each dislocation moves over to the next position, that is by a distance L, the the strain would be as given on the bottom right.



Question is what would be the plastic strain if each dislocation was to glide to the right to place itself at the site of the neighboring disloclocation.

Assume that the spacing between the dislocations is L, and that the spacing between the slip planes is also L.

$$\gamma_P = \frac{b}{L}$$

Now consider that the dislocations move through several multiples, n, of the distance L, so that the distance moved is equal to

$x = nL$

Then the strain would be

$$\gamma_P = \frac{b}{L}n = \frac{bx}{L^2}$$

Write that $\rho = \frac{1}{L^2}$, so that $\gamma_P = \rho x b$ ....(eq). Note that the area density of the dislocations as shown in the sketch on the right, that is the number of dislocations per unit area is given by ρ . You can also show that ρ is also equal to the total line length of dislocations in a unit volume of the crystal.