

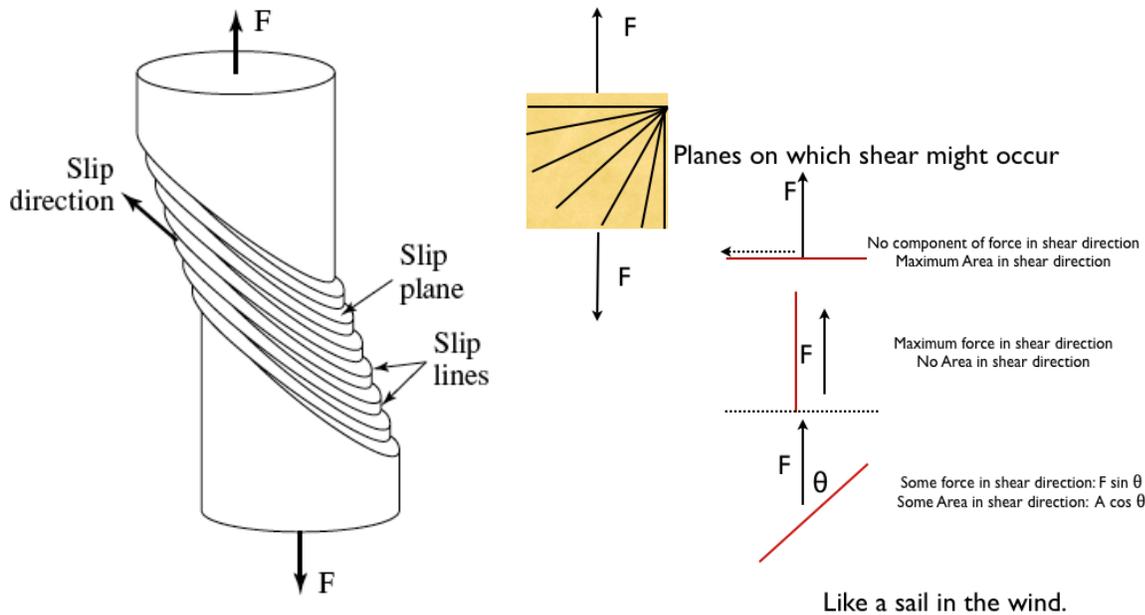
CME 300 Properties of Materials

ANSWERS Homework 2 September 28, 2011

1) Explain why metals are ductile and ceramics are brittle. Why are FCC metals ductile, HCP metals brittle and BCC metals tough?

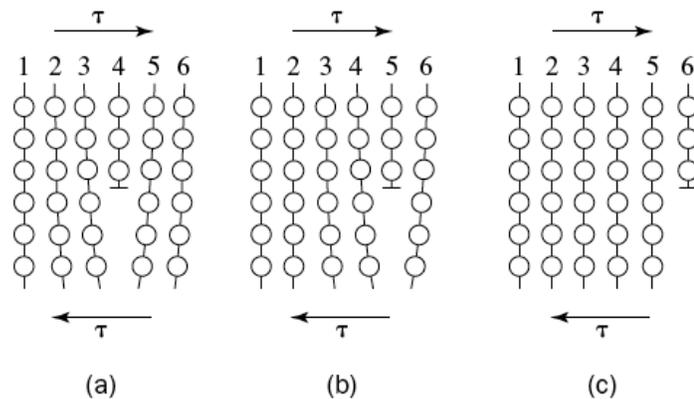
Planes in ceramic crystals cannot slip since this would require dissociation of ionic bonds. When ionic bonds dissociate a crack forms and the material fails in a brittle manner. FCC has 12 slip planes with 4 closest packed planes $\{111\}$ and 3 closest packed directions per plane $\langle 110 \rangle$. HCP has only 3 slip systems. BCC does not have truly closest packed planes so slip must be thermally activated in BCC metals.

2) Why does slip occur along approximately a 45° angle in the following picture?



3) The symbol for a Burgers vector is an upside down T. Explain the meaning of this symbol using an edge dislocation.

FIGURE 3.20. Simplified two-dimensional representation of an edge dislocation and of dislocation movement under the influence of a shear stress, τ , in a single crystalline, cubic-primitive lattice. A $\{100\}$ plane is depicted. The shear stress is shown to be applied parallel to the slip plane and normal to the dislocation line (see Figure 3.21).



The Burgers vector is in the direction of the head of the T, the plane of extra atoms occurs in the stem of the T. Motion of the disclination occurs in the direction of the Burgers vector.

4) Explain strain hardening in an FCC metal like copper.

When an FCC metal is worked, disclinations are introduced. These disclinations interact and pin each other making the metal harder, increasing the yield strength.

5) Why does twinning mostly occur in HCP metals like zinc?

Twinning takes a larger stress than slip along a closest packed plane in a closes packed direction since it involves rearrangement of an entire plane of atoms simultaneously rather than rearrangement of a single row. However, in HCP crystals an insufficient number of slip systems exist so that the second best mechanism to absorb energy is more prevalent.

6) BCC metals display a thermal dependence for the critical resolved shear stress shown in figure 3.23 below. Write an equation for this behavior ($\tau_0 = f(T)$) and explain the terms including a definition of τ_0 . Why do BCC metals differ from FCC and HCP metals in terms of this thermal dependence?

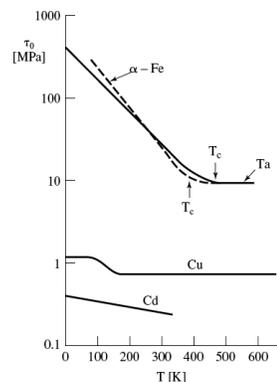
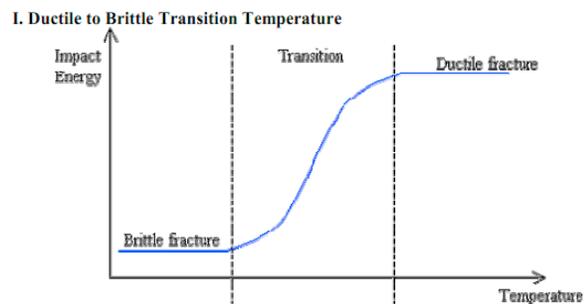


FIGURE 3.23. Schematic representation of the temperature-dependence of the critical resolved shear stress, τ_0 , for Ta (BCC), α -Fe (BCC), Cu (FCC), and Cd (HCP) single crystals. Since τ_0 depends strongly on the crystal orientation, an average orientation has been chosen. Specifically, the tensile direction has about the same angle to the [100], [110], and [111] crystal axes. Note the logarithmic scale on the y axis.



The ductile-brittle transition is exhibited in bcc metals, such as low carbon steel, which become brittle at low temperature or at very high strain rates. FCC metals, however, generally remain ductile at low temperatures.

<http://www.exo.net/~jillj/activities/mechanical.pdf>

τ_0 is the critical resolved shear stress is the shear stress needed to initiate plastic deformation for a crystal. In the figure $\log(\tau_0)$ is linear in temperature up to the critical temperature T_c . For the linear region,

$$\tau_0 = \exp(-K_1 T + K_2)$$

beyond this region a more complicated function is needed. K_2 is the natural log of the critical shear stress at absolute 0, K_1 is the rate of change of the log of critical shear stress as a function of temperature. K_1 is probably related to $k_B/\Delta E$, where k_B is the Boltzmann constant and ΔE is the barrier energy for slip in the BCC system. (Simply adding a constant to the equation in order to mimic the plateau at high T doesn't work with this data.)

BCC does not have closest packed planes. The highest density planes, $\{110\}$, require thermal activation for slip to occur. This involved motion of the atoms about their lattice positions to more or less fill in the gaps making the planes appear to be space filling. The higher the

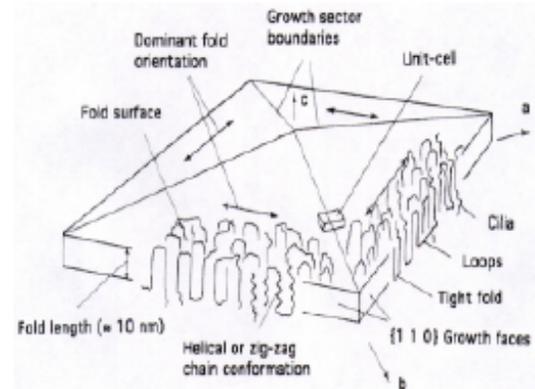
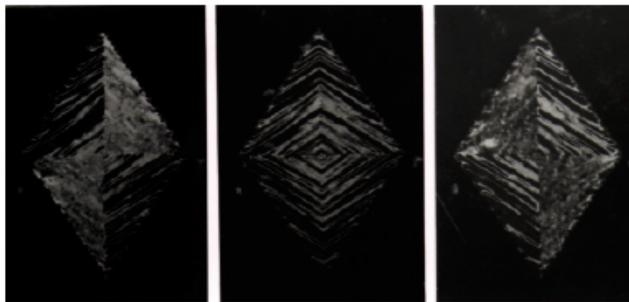
temperature the more the planes appear to be space filling up to the critical temperature. This thermally activated behavior leads to a “brittle to ductile” transition on heating.

7) *Synthetic polymers in the melt are described as random coils, meaning that there is little regular organization of the chain structure. In order for crystallization to occur in these chain molecules what sequence of steps must be followed?*

Polymer chains must form helices and disentangle from the melt in order to be drawn into lamellar crystals. The helices must then diffuse to the growing lamellar edge, nucleate a new plane of chains, chain fold and reinsert into the growing edge.

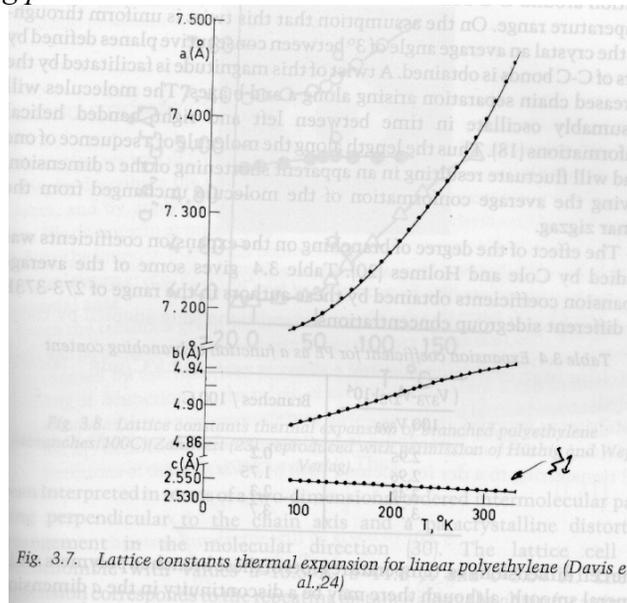
8) *Describe a dilute solution polymer crystal. Why do polymers not crystallize in cubic lattices like metals?*

Polymers crystallize into thin lamellar crystals of about 10 nm thickness and with an aspect ratio similar to a sheet of paper, i.e. with about 1 micron lateral dimensions. In order for chain helices line up normal to the lamellar surface and must fold at the lamellar surface to reenter the crystal. The chains are tilted with respect to the lamellar surface to allow space for chain folding and to relieve tension associated with this fold. This tilt of the chains leads to the formation of edges and pyramid shape for the sheet crystals, similar to a tent. When these crystals are prepared for microscopy the tents collapse in a corrugated manner, as shown in the picture below.



The c-axis in the crystal is the chain helical axis direction. The a and b directions are governed by van der Waals interactions, hydrogen bonding and other weak forces. Since the helix is not symmetric we expect different values for the a and b lattice parameters and the c direction is controlled by covalent bonds so it is quite different than the other two axes. For these reasons polymers never crystallize into cubic crystals.

9) Explain the following plot:



The plot shows the thermal expansion and contraction of the lattice parameters in a polymer crystal. The a and b axis expand in a non-linear fashion due to the complexity of the interactions. The c-axis has a weak thermal contraction that is caused by rubber like elasticity of the chain in the helical axial direction. You can think of the chain as a jump rope that is swinging with thermal excitation. As the temperature rises the rope swings faster leading to an increase in the retraction force at the ends of the chain. This leads to thermal contraction in the c direction of the crystal.

10) Derive the Gibbs-Thompson equation for a cubic crystal such as NaCl. In solution nanoparticles can be made by a chemical reaction that results in a rapid rise in a crystallizing species followed by rapid depletion of the species. Explain this in terms of the Gibbs-Thompson equation.

The derivation is similar to that for the polymer crystal except that there are 6 surfaces to a cubic crystal compared with two high energy fold surfaces in a polymer crystal.

The Hoffman-Lauritzen equation for polymers is derived as follows:

Consider a crystal where $t \Rightarrow \infty$

$$\Delta G_{f,T_{\infty}} = 0 = \Delta H_f - T_{\infty} \Delta S_f$$

$$\Delta S_f = \frac{\Delta H_f}{T_{\infty}}$$

Consider a crystal where t is finite crystallized at $T_{m,t}$ (Gibbs Pseudo-Equilibrium Assumption)

$$V \Delta G_{f,T_{\infty}} = 0 = V(\Delta H_f - T_{m,\infty} \Delta S_f) - 2R^2 \sigma_e$$

$$tR^2 \Delta H_f \left(\frac{T_{m,\infty} - T_{m,t}}{T_{m,\infty}} \right) = 2R^2 \sigma_e$$

$$t = \frac{2\sigma_e T_{m,\infty}}{\Delta H_f (T_{m,\infty} - T_{m,t})}$$

For cubic crystals the third equation becomes:

$$V \Delta G_{f,T_{m,t}} = 0 = V(\Delta H_f - T_{m,\infty} \Delta S_f) - 6R^2 \sigma_e$$

so we have,

$$t = \frac{6\sigma_e T_{m,\infty}}{\Delta H_f (T_{m,\infty} - T_{m,l})}$$

11) A sheet of aluminum is shown below. Explain how the striations in the image are formed and how they relate to the FCC crystal structures we discussed in class.



Each stripe is a grain, a single FCC crystal, that has been drawn out. The grains grow from nucleation sites in the melt and prior to drawing they would be randomly shaped grains similar to that seen in the picture of galvanized steel below.



12) Guess at the origin of the Hall-Petch relationship based on your understanding of yielding in metals. First explain why yielding occurs, then how grains could impact yielding in a polycrystalline sample compared to a single crystal, then indicate a possible origin for the particular functionality in the Hall-Petch relationship, $1/(\text{normalized yield stress})$.

Yielding in FCC metals occurs due to the presence of disclinations and other defects in the crystals. The crystals can absorb energy by motion of these disclinations along slip systems. In a metal sample with small grains some of the grains do not have disclinations since there is a probability per volume that a grain will have a disclination P , so for a given grain the probability that the grain will have a disclination is $P*V = k*P*d^3$. The probability of a given grain having a disclination drops with d . If a grain doesn't have a disclination it has a much higher yield strength. The metal becomes a composite of grains with no disclinations that are hard and brittle and grains with disclinations that are ductile so the overall composite yield strength increases as the grain size decreases for very small grains.

Additionally, defects are trapped at grain boundaries. The probability of a defect encountering a grain boundary in a given time is related to the surface area of a grain, d^2 , the number density of

grains, $V_{\text{sample}}/V_{\text{grain}} \sim 1/d^3$ and the rate and time of grain diffusion, r and Δt . The rate of disclination trapping at grain boundaries should go with $1/d$. The more trapping of disclinations the higher the yield stress so a sample with smaller grains should have a larger yield stress.

The Hall-Petch relationship is an empirical function (based on experimental observation). The calculation of yield stress is a fairly complicated and ill-defined problem but we can at least list some reasons for an increase in yield stress with decreasing grain size.

The following is an explanation from <http://www.exo.net/~jillj/activities/mechanical.pdf>

A change in grain size affects the yield strength due to the dislocations interacting with the grain boundary as they move. The boundaries act as obstacles, hindering the dislocation glide along the slip planes. As subsequent dislocations move along the same slip plane the dislocations pile-up at the grain boundaries.

The dislocations repel each other, so as the number of dislocations in the pile-up increases the stress on the grain boundary increases. In fact, if there are n dislocations in the pile-up, the stress at the grain boundary will be n times the applied stress.

If the grain boundary in a sample gives way at a stress t , there needs to be a stress of t/n applied to the sample in order to cause the boundary to collapse.

In a larger grain there will be more dislocations within the grain, so there will be more dislocations in the pile-up. Therefore a lower applied stress is required to produce a local stress great enough to cause the grain boundary to collapse. Accurate modeling is difficult, but it is found that the tensile yield strength, $Y.S$, and hardness, H , are related to grain diameter, d , by the *Hall-Petch equation*: