Midterm Exam

October 18, 2011

Name: SOLUTION

Prob. #1
Prob. #2
Prob. #3a
Prob. #3b
Prob. #4
Prob. #5
Total

Instructions: Answer all questions on the examination sheets. (use backs if needed)
Calculators Allowed but No Books & No Reference Sheet. Time: 75 minutes.
1. (15 pts) In a brief essay, describe how chemical reactions that occur between gaseous species can be speeded up (catalyzed) by providing surfaces on which the reaction can occur and why some materials might be better catalysts than others.

Reactions between molecules or atoms require them to collide with enough thermal energy to get past the energy barrier for the reaction. In gas phases, this means they are cruising around in three dimensions and only hit each other rarely. By placing a surface in the gas, the species hit the surface and stick to it. While they are sticking to it, the other species do the same and this reduces the dimensionality of the search. It is easier for the species to find each other and react. If the surface has features such as ledges and steps, these serve to capture the reactants, localizing them so that the search becomes along one dimensional lines on the surface, reducing the dimensionality of the search even more and dramatically speeding up the number of times per second that the reactants hit each other. This is the essence of catalysis. This is a complete answer worth 15 points.

Now, more recently, such as at the ECS meeting that I attended in Boston, people are learning that the details of the “cradles” in which the reactants find themselves can also influence the reaction speed. In particular one of the biggest challenges in Materials Science for the 21st century is to create efficient and effective catalysts for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) which are the limiters for high performance batteries. Researchers have learned (in 2009 it became widely appreciated) that modifying the lattice parameter of a catalyst by alloying it with other metals modified the fit for oxygen, modified the d shell electron energies so they were more in line with what oxygen needed for ORR and OER, and had some synergistic effects by having localized regions of different metal types to help break or form the Oxygen molecules. The sluggishness of this reaction is the main road block to having fantastic batteries that are 5 times better than current Li-ion technology….the Li Air battery. If you are interested in research on this topic, I would love to talk to you.
2. (25 pts) Materials Scientists need to be able to characterize the internal structure of a material to understand its properties. This is the definition of materials science...the study of the relationships between the microstructure and the material properties. Often they do this by looking at it at magnification using an optical microscope. But if you ask the machine shop to cut your sample, the surface will be intrinsically damaged. In fact, no matter how you cut it, the surface will not be the same as the inside. In a two part essay, here and on the next page, explain the logic and process for obtaining a flat two-dimensional cross section and how to best examine this section to learn about the grain size.

**Creating a Damage Free Surface:**

To create a damage free surface, we need to assess how deep the damage is. That is, we need to determine how deep into the surface the stresses from the cutting operations extended in terms of dislocations, phase transitions, cracking, etc. Any type of damage. Usually this can be done by doing cross sections where you look at the microstructure from the side. Take two specimens and put them face to face in a specimen mount, like we did in the lab, and then polish them a very large amount so that you are sure you have exceeded the damage depth.

Use a rule of threes by taking off three times the depth of material equal to the size of the abrasive and then make the abrasive smaller and smaller until you have removed more than the total depth you found from the cross sectioning. All this gets you down to a damage layer, after you use diamond abrasives or aluminum oxide abrasives that is in the micron range where you can etch the surface to chemically remove the last little bit.

Now the rule of threes is maximally conservative...use this when you truly don’t know how deep the damage process is. Once you have worked with a given material for a while, you can figure out how deep the damaged layers are....some steels only have damage equal to the abrasive size....some have damage less than the abrasive size. Because harder materials allow less damage, the harder the material, the easier they are to do a good job polishing.
Observing and Measuring the Grain Size:

Once you have a flat surface (flat is needed to get good results with the microscope so everything is in focus) etching the surface reveals the microstructure. This is because the first etching removes the last of the damaged layer from the finest abrasives. More etching preferentially attacks the microstructure dissolving grain boundaries more deeply, or attacking grains with different orientations to produce different surface pitting patterns. Basically, you are looking to produce a geometrical surface variation that reflects light differently. In some materials, the oxides that form on the surfaces interact with light via polarization variation so that a polarizer/analyzer in the optical path allows different regions to have different light levels (darker or brighter).

Usually, the grain boundaries look black because there are inclined regions so that light bouncing from them does not go back into the lens. Recall that a perfect lens takes uniform illumination from a mirror like surface and creates a uniformly bright surface. Regions where light is missing look dark.

On the image of a photo, we can measure the grain size by counting.

One method just compares typical grain size images with the one you are observing and getting an estimate “at a glance” Special eyepieces have this comparison facilitated by arranging the various comparative micrographs around the perimeter.

Or, you can draw lines on the photograph and count the intersections with a total amount of line to get a good average. It is good to use circles to remove bias of directions, as the grain size may be directionally different. You can also align the lines parallel to the principal directions to determine grain size in these directions.

Lastly, you could simply count the number of grains in a specific area in a 100X photo and follow the rules for the ASTM grain size measurement. If your photo is at a different size, you scale the area that you count as if it were 1 in squared on a 100X photo.

Many material properties depend on grain size so it is useful to plot things like yield stress, elongation, optical transmissivity, etc vs grains size.
3a. (10 pts) Explain the logical processes that enable you to use a hardness test to estimate the ultimate tensile strength of a metal and how you would do it.

A hardness indentation deforms some parts of the dented region a lot and other portions only a little. In some sense, the indentation process is a means of averaging different parts of the stress strain curve in a weighted manner based on how much of each type of deformation occurs. Thus, if the shape of the stress strain curve is the same, only the UTS is changing, it is reasonable to expect an excellent correlation between UTS and hardness. Experiments have shown this correlation over the years so now we can proceed with confidence to use hardness as a proxy for a full stress strain test based on the correlations.

3b. (10 pts) An FCC metal has a density of 2.7 g/cm³ and an atomic weight of 27 amu. Another FCC metal has a density of 8.96 and an atomic weight of 63.5. Calculate the lattice parameters and compare them. Is it reasonable that they will be similar or different.

There are 4 atoms per cell for FCC. Atomic weight is in units of grams/mol and Avagado’s number is atoms per mole. So we arrange it to find the lattice parameter in units of cm for a cubic cell

\[
\text{cube root}(\frac{(4 * 27)}{6.02e23} / 2.7) = 4.05030598 \times 10^{-8}
\]
\[
\text{cube root}(\frac{(4 * 63.5)}{6.02e23} / 8.96) = 3.61112957 \times 10^{-8}
\]

Note that the values are not very different. In fact they are very similar and this is reasonable because the inner electron structures of metals are all very similar, with the spherical inner electrons all being similar. The metal cations look like cations of 1, 2 or 3 valence. As metals, the outer electrons are in the “sea of electrons” Most metals have very similar lattice parameters with far less variation than might be expected from their atomic weights.
4. (20 pts) Answer the following short answer questions with T or F.

a. T Window glass can be considered an inorganic polymer.

b. T Putting small molecules in otherwise glassy polymers makes them more flexible.

c. T Orthorhombic crystal structures have all three lattice parameters with different values.

d. F A spherulite is a region in a polymer where the local structure is 100% crystalline.

e. T Grain boundaries disturb the motion of electrons, the motion of dislocations, the motion of vacancies, the motion of heat, and the motion of light.

f. F Atoms with spherically symmetric electron densities do not attract other atoms which is why they are called inert gasses.

g. T Metals can be considered to be fuels because energy was stored in them when they were processed from the ore.

h. T Dislocation tangles in metals caused by deformation that are responsible for strengthening metals can be removed by waiting, if you wait long enough.

i. T It is reasonable to expect cast alloy parts to have larger variability in properties than wrought alloy parts.

j. F Plastic deformation weakens metals.
5. (20 pts) Fill in the blank or complete the phrase with one or more words to make a true statement.

a. When the side groups of a polymer are all on the same side of the molecule, the structure is said to be ____ISOTACTIC______.

b. The molecular weight of a polymer can be computed as both a weight averaged molecular weight and a ____NUMBER______ averaged molecular weight.

c. A Frank-Read source is a mechanism by which ____DISLOCATIONS ARE GENERATED____.

d. At room temperature, atoms typically move with a vibrational amplitude that is _10____% of the average inter-atomic spacing.

e. Steady state diffusion implies a concentration of the diffusing species that depends ____LINEARLY____ on the dimensions of the sample.

f. You would expect the fractured surface of a diamond to become covered with impurities because ____FREE RADICALS CREATE COVALENT BONDS WITH H, C, O, ETC____ the covalent bonds need to be terminated.

g. Bragg’s law is \( n\lambda = 2d \sin(\theta) \). Sketch a diagram below that shows the incident x-ray beam, the diffracted beam, and parallel lines representing the planes of spacing \( d \). Label the underlined items in your sketch.

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incident

\( \theta \)

\underline{diffracted}

\underline{Planes}
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h. In the sketch above, label the angle \( \theta \).

i. If polymers are viscous at high temperature, as they cool, the become rubbery, then ____LEATHERY____, and a the lowest temperatures, they are characterized as ____GLASSY____.

j. Metals are more ductile than ceramics because the bonding of metals HAS EVERY ATOMS BONDING TO ALL OTHERS____ while the bonds in ceramics ____ARE DIRECTIONAL AND DO NOT ACCEPT SLIP IN ALL DIRECTIONS____.