Department of Materials Science and Engineering
Massachusetts Institute of Technology
3.14 Physical Metallurgy – Fall 2003

Solutions to Problem Set #8

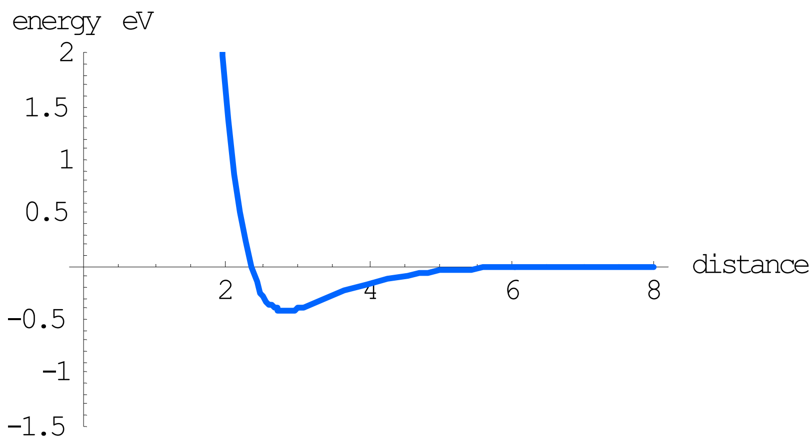
8.1 *It is possible for zinc crystals to undergo very large plastic strains at temperatures below room temperature. This is not true in polycrystalline zinc, which normally shows a very low ductility at sub-ambient temperatures. Give an explanation for this fact based on the mechanical properties of zinc.*

Zinc is a metal that deforms very easily by basal slip at a very low level of stress even at low temperatures. In other words, it deforms readily by easy glide and the work hardening rate is low. At the same time, slip on other slip planes in zinc becomes increasingly more difficult the lower the temperature. In a single crystal of zinc, easy glide is effectively unrestricted because the shear along the slip planes in unimpeded at the free surfaces of the crystal. However, in a polycrystalline metal, the slip planes do not end at a free surface, but rather at a grain boundary, where the basal plane of the next grain is not normally aligned so as to pass the shear into the next grain. Compounding this problem is the fact that zinc cleaves easily along its basal plane at low temperatures. Thus, the high stress that develops at the grain boundaries due to the inability of the basal slip to be accommodated between grains leads to brittle cleavage or intergranular fracture.

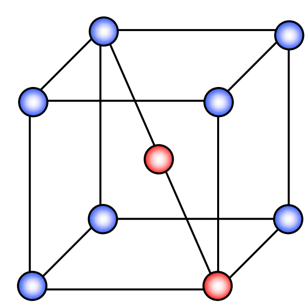
8.2 The first step is to determine the energy-separation curve for Fe.
a. Plot the interatomic potential for Fe.
b. Identify the mean interatomic distance across the fracture plane (100) at zero stress (in class we called this r_o, your book calls it d).

a. Using Mathematica…
α_{Fe} = 1.3885 Å
r_{Fe} = 2.845 Å
D_{Fe} = 0.4174

$$\text{IronEnergy} = D_{Fe}\left(e^{-2\alpha_{Fe}(r-r_{Fe})} - 2e^{-\alpha_{Fe}(r-r_{Fe})}\right)$$



b. The interatomic spacing across the fracture plane, d, is just going to be ½ of the lattice parameter (as calculated by this potential) since the cleavage plane is (100). The parameter r_o gives the distance between the two red atoms in the figure here. Some simple geometry then tells us that the lattice parameter $a = \frac{2r_o}{\sqrt{3}}$, and d = a/2, or **d = 1.642 Å**.



8.3 The next step is to determine the properties of the cleavage plane.
a. Calculate the bond density in the fracture plane.
b. Calculate the surface energy for the (100) plane (= γ). Hint: This is the energy of all of the bonds that must be broken to create this surface.

a. Let's assume that r_o is twice the radius of the atom (distance between the centers of two atoms in the hard sphere model). Then the atomic radius of Fe is 1.422 Å. The bond density, or atomic density, in the (100) plane is given by number of bonds/area of plane or:

$$\frac{4}{a^2} = \frac{4}{(3.285\text{Å})^2} = 3.706 \times 10^{19}\,\text{m}^{-2}$$

b. Surface energy should be in J/m^2 – energy per unit area. For our unit area, we will take the area of the (100) face of the unit cell, 1.079 x 10^{-19} m^2. There is one total atom in each (100) face, which will have to lose bonds with its 4 NN (distance r_o), 1 NNN (distance 2/sqrt3* r_o) and 4 NNNN (distance 2 r_o). That will be enough neighbors to consider. The total energy is then:

$$\text{FeSurfaceEnergy} = 4D_{Fe}\left(e^{-2\alpha_{Fe}(r_{Fe}-r_{Fe})} - 2e^{-\alpha_{Fe}(r_{Fe}-r_{Fe})}\right) + \cdots$$
$$\cdots + 4D_{Fe}\left(e^{-2\alpha_{Fe}(2r_{Fe}/\sqrt{3}-r_{Fe})} - 2e^{-\alpha_{Fe}(2r_{Fe}/\sqrt{3}-r_{Fe})}\right) + 4D_{Fe}\left(e^{-2\alpha_{Fe}(2r_{Fe}-r_{Fe})} - 2e^{-\alpha_{Fe}(2r_{Fe}-r_{Fe})}\right)$$

This equals -2.06339 eV. Dividing by the area and converting from eV → J, we find the surface energy to be **3.06 J/m^2**. (If we had used only first NN, it would be ~2.5 J/m^2).

8.4 Finally, calculate the theoretical fracture stress for cleavage for two different scenarios:
a. With no flaws present
b. With a 5 μm long Griffith crack (Figure 22.3). This is about the smallest size crack that you could detect with an optical microscope. The microscope will not tell you the radius of curvature at the tip, so you will need to make a reasonable assumption for it.

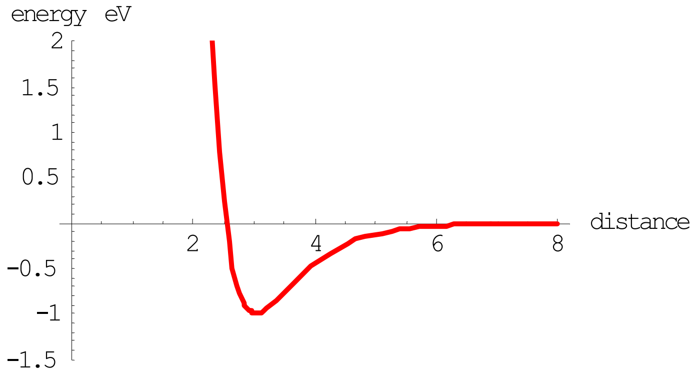
a. With no flaws, the theoretical fracture stress is $\sigma_{th} = \sqrt{\frac{\gamma E}{d}}$. Plugging everything in (E_{100} of Fe = 125 GPa), we find $\sigma_{th} = \sqrt{\frac{3.06 J/m^2 \cdot 125\times10^9\, Pa}{1.642\times10^{-10}\, m}}$ = **48 GPa**

b. With a crack, $\sigma_{th} = \left(\frac{\gamma E}{4a}\left(\frac{\rho}{d}\right)\right)^{1/2}$. Assuming the crack is atomically sharp (close to the truth with such a small crack), ρ will be ~5Å.

$$\sigma_{th} = \left(\frac{3.06 J/m^2 \cdot 125\times10^9\, Pa}{4\cdot 2.5\times10^{-6}\, m}\left(\frac{5\times10^{-10}\, m}{1.642\times10^{-10}\, m}\right)\right)^{1/2}$$ = **341 MPa**

8.5 Repeat the calculations (interatomic distance, surface energy, and theoretical fracture stresses) for tungsten. Compare your results to those for Fe and explain the reason for any differences you find.

a. Potential looks like:
$\alpha_W = 1.4116$ Å
$r_W = 3.032$ Å
$D_W = 0.9906$



b. Interplanar spacing: $a = \frac{2r_o}{\sqrt{3}}$, then d = a/2, or **d = 1.750 Å**.

c. Cleavage plane bond density: $\frac{4}{a^2} = \frac{4}{(3.501\text{Å})^2} = 3.26 \times 10^{19}\,\text{m}^{-2}$.

d. Surface energy: area of (100) face = 1.226 x 10^{-19} m^2. Energy of 4 NN, 1 NNN, 4 NNNN = -4.89266 eV. The total surface energy is **6.30 J/m²** (~5.2 J/m² considering only NN).

e. No flaw fracture stress: $\sigma_{th} = \sqrt{\frac{6.30 J/m^2 \cdot 385 \times 10^9\, Pa}{1.750 \times 10^{-10}\, m}}$ = **118 GPa**

f. With a crack: $\sigma_{th} = \left(\frac{6.30 J/m^2 \cdot 385 \times 10^9\, Pa}{4 \cdot 2.5 \times 10^{-6}\, m} \left(\frac{5 \times 10^{-10}\, m}{1.750 \times 10^{-10}\, m} \right) \right)^{1/2}$ = **832 MPa**

Both the surface energy and modulus are significantly higher in W than Fe, and therefore he theoretical fracture stresses are also much higher with and without a flaw.