3.22 Mechanical Properties of Materials Spring 2008

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## Problem Set #4

Due: Tuesday, April 15 by 5:00 PM

1. A non-planar dislocation loop is shown in the diagram below. Each of the dislocation segments lies parallel to one of the coordinate axes. The segment AB is a left-handed screw dislocation.



- (a) Identify the character (positive edge, negative edge, right-handed screw (RHS), lefthanded screw (LHS)) of each segment of the dislocation loop.
- (b) A positive shear stress  $\tau_{zx} = \tau_{xz}$  is applied. Indicate the direction of the Peach-Koehler force for each segment, and list those segments for which the force is zero.
- 2. Solute strengthening includes a point defect-based obstacle to dislocation motion, where this obstacle is an impurity or solute atom in the "host" or "matrix" crystal lattice. Those taking 3.21 in parallel have already considered the equilibrium situation of a solute atom interacting with an edge dislocation self-stress field (Balluffi, Allen & Carter, Kinetics of Materials; Section 3.5.2). Here, we will continue the kinetic consequences of this analysis.
  - (a) Assume a point defect to be well-represented by an elastic sphere of effective radius  $r(1 + \delta)$ , where r is the radius of the host lattice (or matrix) atom and  $\delta$  is the positive/negative difference between the solute and matrix atomic radii. Note that  $\delta$  is positive if the solute atom exceeds the host atom in size; and negative if the solute atom is smaller. Assuming the atomic size mismatch is sufficiently small, let the solute atom be a substitutional impurity in the lattice, and express the change in volume at that lattice site  $\Delta V$  due to replacing a lattice vacancy (the volume of the missing atom in the host lattice) with a solute atom, in terms of the solute atom radius and induced strain  $\epsilon$ .
  - (b) Cottrell considered the equilibrium position or "atmosphere" of the solute atom due to the self-stress of a dislocation, as a function of distance from the dislocation core. In general, the elastic strain energy  $U_e$  of the crystal increases as a  $p\Delta V$  term, where pis equal to the hydrostatic stress acting on that point-defected volume  $\Delta V$ . Using the elastic solutions to dislocation self-stress and the definition of hydrostatic stress, graph the hydrostatic isostress contours as a function of (x, y) or (r,  $\theta$ ) distance around both an edge dislocation core and around a screw dislocation core. (Mathematica, Matlab, etc. are handy rendering programs for analytical equations.) Here, you can use the required

structural and elastic constants for bcc (also called  $\alpha$ -phase) Fe. Cottrell combined all these structural/elastic terms into a constant, such that  $U_e$  was reduced to a material-dependent constant modifying a dependence on just  $\theta$ ! and r.

- (c) From the above graphs, show the most energetically stable location of a smaller solute atom like C in terms of  $\theta$ , the angular position defined by your coordinate system at the edge and screw dislocation cores. (Aside: Note that the above analysis was for a substitutional atom, but C is in fact an interstitial defect in Fe; this point is usually neglected in analysis of point-line defect interactions, but does affect the number of lattice points available to both species.)
- (d) The equilibrium or steady-state concentration of solute atoms as a function of distance from the dislocation core can be predicted from thermodynamics, based on an Arrhenius dependence on the core-distance-dependent energy barrier  $U_e$ . Predict this concentration at a location (0, -b) from the core of a positive edge dislocation in Fe at room temperature (300 K), assuming that the concentration of C solute far from the dislocation is 0.1% and that the binding energy of C to the edge dislocation core is 0.5 eV. Explain implications in terms of distribution of the C solute within the Fe lattice.
- (e) Cottrell considered these interactions even before dislocations were observed, so he analyzed the effect of any applied pressure on the solute atom. Use Peach-Koehler to take the opposite view: What is the driving force for glide and/or climb due to the hydrostatic pressure created by the solute atom that is located at (0, -b) from a positive edge dislocation core and from a positive screw dislocation core?
- (f) Now as the dislocation glides under applied shear stress on its slip plane, the role of C in solute strengthening depends on a competition between solute diffusion (keeping up with the core) and maintained dislocation velocity. For example, if diffusion times/distances are comparable to glide times/distances, the C will keep up with the core and continue to impede glide. This is called dynamic strain aging, and leads to serrated yielding in unaxial tension (stress above yield point dropping as dislocations break free of solute; and increasing as solute diffuses back to the core. How fast/far is that? Here, we make analogy to Cottrell's classic strain aging argument, which showed scaling between the time required for a moving solute atom to diffuse into a stationary dislocation core (opposite case to our dynamic strain aging), show how the concentration or number of solute atom obstacles at the bcc Fe dislocation core depends on the diffusion time *t* of the C solute (see BAC's KoM). Then compare this time for a solute atom to diffuse a distance  $|\mathbf{b}|$  with the time it takes for a dislocation to move a distance  $|\mathbf{b}|$  for a typical metal (see your Orowan strain rate solution from PS3).
- 3. We discussed how two edge dislocations could intersect, resulting in an edge-type jog in one of them. Show whether it is possible for pure (edge or screw) dislocations to intersect in such a way that would result in formation of a sessile kink in either of the two dislocations. These could be two edges, two screws, or one edge/one screw.
- 4. You are given an Al- 2 at.% Cu alloy where the Cu is in solution with the Al. Your boss then asks you to make the material as strong as possible.
  - (a) Before you do anything to the material, first estimate the amount of solute (in at.%) necessary to put one solute atom at each site along all of the dislocations in the sample.

This will give you an idea of how much solute is necessary to strengthen the material by solute alone.

- (b) If you anneal the alloy at 400 °C, schematically show a plot of temperature vs. time, particle size r vs. time, particle spacing L vs. time, and yield strength vs. particle size. (Treat any additional equilibrium phases in a continuum manner ignoring interfaces and atomic structure.) In the last plot, describe the different strengthening mechanisms, including relative magnitudes, the would be the effective mechanisms at different times.
- (c) Suppose instead of an alloy, you started with a composite of Al with  $Al_2O_3$  particles dispersed in it. (Assume the volume fraction of the particles is the same as the particles in part (b).) How would you expect the maximum yield strength to change and the particle size r at which this maximum occurs to change relative to the metal alloy case? Show this on a yield strength vs. particle size graph for both materials.
- 5. No new wiki work before Quiz 2; will resume in PS5. Where are we going with this? Each team will present a 15 minute discussion of the special topic during lecture at the end of the term, summarizing key mechanical behavior topics covered in the wiki over the term. Three of these topics will be chosen at random to be included on Quiz 3, and you'll answer 2 of them (one cannot be from your own team). You may want to start discussing how you'll plan to do this short presentation.