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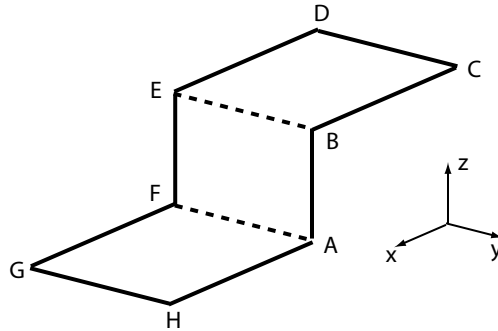
3.22 Mechanical Properties of Materials
Spring 2008

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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), left-handed screw (LHS)) of each segment of the dislocation loop.

Solution: Since we are told AB is LHS, we know the burgers vector \mathbf{b} is parallel to the line vector \mathbf{s} but in an opposite direction. This sets \mathbf{s} for the other segments in the loop; it goes counterclockwise around the loop. The burgers vector for the loop does not change. This gives The convention for a positive and negative edge dislocation is

Segment	Character
AB	LHS
BC	- Edge
CD	- Edge
DE	+ Edge
EF	RHS
FG	+ Edge
GH	+ Edge
HA	- Edge

arbitrary in any real sense; we can choose to define a positive edge with a Burgers vector to the right for a dislocation line direction into the page, but we cannot choose to make these vectors non-orthogonal (that is the defining property of the edge dislocation). Which ones you choose to call positive and negative are immaterial, as long as you recognize that DE and GH are opposite; and BC and HA are the same and opposite from DE and FG .

- (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.

Solution: This can be easily determined from the Peach-Koehler equation

$$\frac{\mathbf{F}}{L} = (\mathbf{b} \bullet \bar{\boldsymbol{\Sigma}}) \times \zeta$$

The stress state given is

$$\bar{\boldsymbol{\Sigma}} = \begin{vmatrix} 0 & 0 & \tau_{xz} \\ 0 & 0 & 0 \\ \tau_{xz} & 0 & 0 \end{vmatrix}$$

*Let's look at **BC** which has a line vector $\zeta = [\bar{1}00]$. The Burger's vector of loop $\mathbf{b} = [00\bar{1}]$. With this information, we calculate the dot product of \mathbf{b} and $\bar{\boldsymbol{\Sigma}}$ and take the cross product with ζ to get*

$$\frac{\mathbf{F}}{L} = (\mathbf{b} \bullet \bar{\boldsymbol{\Sigma}}) \times \zeta = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -\tau & 0 & 0 \\ -1 & 0 & 0 \end{vmatrix} = \mathbf{0}$$

*So there are no forces acting on **BC** due to the applied stress state. If we do a similar analysis for **DE**, **FG**, and **HA** we find that these segments also experience no force.*

*Let's look at **AB** which has the same Burger's vector and experiences the same applied stress, but $\zeta = [001]$. Calculating the forces for acting on this segment from Peach Koehler yields*

$$\frac{\mathbf{F}}{L} = (\mathbf{b} \bullet \bar{\boldsymbol{\Sigma}}) \times \zeta = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -\tau & 0 & 0 \\ 0 & 0 & 1 \end{vmatrix} = [-\tau\mathbf{00}]$$

*Therefore the force acting on this segment is in the negative y-direction. A similar analysis can be done for **CD**, **EF**, and **GH**. The results are summarized in the table below.*

Segment	Force direction
AB	- y
CD	- z
EF	+ y
GH	+ z

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 δ is the positive/negative difference between the solute and matrix atomic radii. Note that δ 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 ΔV 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 ϵ .

Solution: The volume of the vacancy is $\frac{4}{3}\pi r^3$ and the volume of the solute atom is $\frac{4}{3}\pi r^3(1 + \delta)^3$. In this case, δ is the strain due to putting an atom in the vacancy ϵ . The change in volume is thus written as

$$\Delta V = \frac{4}{3}\pi r^3(1 + \epsilon)^3 - \frac{4}{3}\pi r^3$$

Because ϵ is small, higher order terms from the expansion of $(1 + \epsilon)^3$ will be negligible and we can write

$$\Delta V = \frac{4}{3}\pi r^3\epsilon$$

- (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 p is equal to the hydrostatic stress acting on that point-defected volume ΔV . 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, θ) 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 α -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 .

Solution: The elastic strain energy normalized by line length L is

$$\begin{aligned} \frac{U_e}{L} &\simeq p\Delta V \\ &\simeq \sigma_H\Delta V \\ &\simeq \frac{-1}{3}(\sigma_1 + \sigma_2 + \sigma_3)(\Delta V) \end{aligned}$$

For a screw dislocation, $U_e/L = 0$ because there is no hydrostatic component in its self energy. In the case of an edge dislocation however, we substitute the hydrostatic stress in the above equations σ_H with the self stress of the dislocation such that

$$\frac{U_e}{L} = \left[\frac{2}{3}(1 + \nu) \frac{Gb}{2\pi(1 - \nu)} \frac{y}{x^2 + y^2} \right] (\Delta V)$$

Substituting the change in volume we calculated in part (a), we get

$$\frac{U_e}{L} = \left[\frac{2}{3}(1 + \nu) \frac{Gb}{2\pi(1 - \nu)} \frac{y}{x^2 + y^2} \right] \left(\frac{4}{3}\pi r^3\epsilon \right)$$

Although we can plot the elastic strain energy in a cartesian coordinate system using this equation, we can also switch it to polar coordinates and plot it as

$$\begin{aligned}\frac{U_e}{L} &= \left[\frac{4(1+\nu)}{9(1-\nu)} Gb \right] \left(\frac{\sin \theta}{r} \right) (r^3 \epsilon) \\ &= AGbr^3 \epsilon \frac{\sin \theta}{r} \\ &= K \frac{\sin \theta}{r}\end{aligned}$$

Writing it in this way, we condense all the material parameters in the factor K and can therefore calculate the elastic strain energy at any point (r, θ) around the dislocation core. For Fe, $G \sim 70$ GPa, $b \sim 0.3$ nm, $\nu \sim 0.3$, $r \sim 0.15$ nm, and

$$\begin{aligned}\epsilon &= \frac{r_{\text{Fe}} - r_{\text{C}}}{r_{\text{Fe}}} \\ &= 0.43,\end{aligned}$$

making $k = 1.4 \times 10^{-29}$ N m². The graph of the hydrostatic isostress contours around an edge dislocation is shown in Hull and Bacon, Fig. 10.11 very schematically (this is the fig reproduced in KOM), and the normal stress component σ_{zz} is shown in Hull and Bacon, Fig. 9.10

- (c) From the above graphs, show the most energetically stable location of a smaller solute atom like C in terms of θ , 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.)

Solution: A small atom like C is stable at $(0, -b)$ (below the dislocation core) because the largest tensile stress state is located there. The C atom, which has a compressive stress state associated with it, can reduce the energy of the system by moving to this position.

- (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.

Solution: An Arrhenius relationship for the steady-state concentration gradient based on the energy barrier U_e (we are now ignoring writing the L and calling this the elastic

strain energy per unit length) we examined in part (b) can be written as

$$c(x, y) = c_o \exp \frac{-U_e}{k_B T}$$

where c_o is the global concentration of the solute (give as 0.1%), T is the temperature (given as 300 K), and k_B is Boltzmann's constant. At (0,-b)

$$U_e = 10^{-29} \left[\frac{\sin(0)}{|-b|} \right] = 0$$

Therefore, $c(0, -b) = c_o = 0.001$, which implies that all the carbon will be at the dislocation core (which is given by (0,-b)). This is nonsensical. Suppose instead that $\theta = 270^\circ$,

$$\begin{aligned} U_e &= 10^{-29} \left[\frac{-1}{0.3 \text{ nm}} \right] \\ &= 3 \times 10^{-20} \frac{\text{J}}{\text{atom}} \\ &= 0.2 \frac{\text{eV}}{\text{atom}} \end{aligned}$$

which gives us $c = 3.6 \times 10^{-7} = 3.5 \times 10^{-5}\%$. This means that all the carbon atoms are not actually at the dislocations, or stated another way, only a fraction of the carbon atoms are at the dislocation core.

- (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?

Solution: The Peach-Koehler equation is

$$\frac{\mathbf{F}}{L} = (\mathbf{b} \bullet \bar{\Sigma}) \times \zeta$$

The presence of a solute atom creates a hydrostatic stress state such that

$$\bar{\Sigma} = P = -\frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3)$$

where σ_o is the stress due to the solute replacement of the lattice site. In the case of an edge dislocation, we can say

$$\begin{aligned} \zeta &= [010] \\ \mathbf{b} &= [100] \end{aligned}$$

and

$$\mathbf{b} \bullet \bar{\Sigma} = \left[\begin{array}{c} -\sigma_o \\ 3 \\ 00 \end{array} \right]$$

giving

$$\frac{\mathbf{F}}{L} = \left| \begin{array}{ccc} \hat{i} & \hat{j} & \hat{k} \\ -\frac{\sigma_o}{3} & 0 & 0 \\ 0 & 1 & 0 \end{array} \right|$$

The only non-zero force therefore is in the k -direction, which is to say it is a “climb” force.

In the case of a screw dislocation, we can say $\zeta = [100]$ and $\mathbf{b} = [100]$. With the same $\bar{\Sigma}$ as above, we find that all forces are zero.

- (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 uniaxial 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).

Solution: See KoM pg. 73 Ex 3.9, which gives a development of these equations based on our stated assumptions. You can reproduce this series of steps, but the point here is to translate the symbols and terms into those we’ve used in 3.22 so that you can be sure you understand the result in both contexts (one with an emphasis on kinetics, the other with an emphasis on mechanics).

The key result is that carbon diffuses along tangents to the isostress contours around the dislocation – a roughly circular loop that is everywhere tangent to the isostress lines. This results in a velocity \mathbf{v} related to the diffusion distance R by

$$\mathbf{v} \sim \frac{1}{R^2}$$

Therefore, the diffusion time is simply the diffusion distance $2\pi R$ around that tangent contour, or

$$t \sim \frac{2\pi R}{1/R^2} \sim R^3$$

so R goes as $t^{1/3}$.

Next, the volume of solute V within a circle of radius R is

$$dV \sim \int_R^\infty \langle v \rangle dR dt \sim \frac{1}{R} dt$$

The number of solute atoms N in this circle at time t is then

$$N \sim \int_0^t \frac{1}{R} dt \sim \int_0^t \frac{1}{t^{1/3}} dt \sim t^{2/3}$$

This is the solute/time relation, which indicates that the amount of time it takes for the solute to diffuse back to the dislocation core depends in part on the solute concentration.

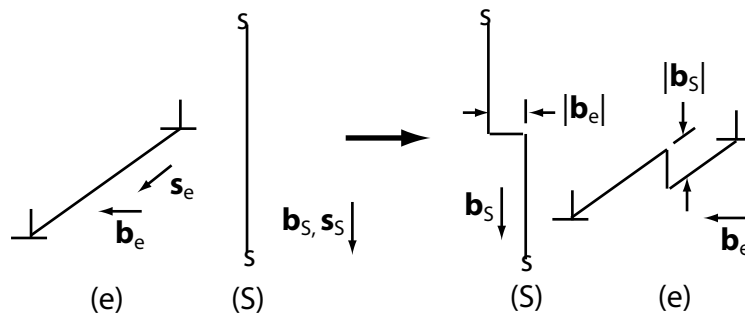
To determine a glide time, we can recall from PS3 that typical dislocation velocities are 10 cm/s, so for a glide distance of one Burgers vector = 0.3 nm (estimate), $t = b/v = 3$ ns.

To determine a diffusion time, we could assume steady-state diffusion such that $t = x^2/4D$, where x is diffusion distance of one Burgers vector and D is the diffusivity of C in bcc Fe. This has been tabulated in various papers and textbooks; I adopt the expression listed in Tibbets, *J. Appl. Phys.* 51: 4813 (1980), which I found via a Google Scholar search and then confirmed on the journal site: $D = 0.47 \exp(-1.6C) \exp([-37,000 - 6600C]/RT) \text{ cm}^2/\text{sec}$ where C is at.% carbon. Then for $b = 0.3$ nm (an estimate), $T = 300$ K (room temp), and 0.1 at.% C (given), $D = 1.8 \times 10^{-28} \text{ cm}^2/\text{s}$, and thus $t = 2.9 \times 10^{11} \text{ s}$. This is a very long time, in fact it would require precisely 9218 years to attain this diffusion distance at room temperature. Indeed, we need to deform materials like this simple steel at temperatures $T \sim T_{\text{melt}}$ to observe this dynamic strain aging.

The temporal mismatch between glide and diffusion at room temp here is real, and underscores the strong Arrhenius dependence of diffusion required for serrated yielding and dynamic strain aging to be observable.

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.

Solution: See figure below (note that \mathbf{s} represents the line vector ζ). When the edge and screw dislocations intersect, a jog with edge character and length $|\mathbf{b}_S|$ is created in the edge dislocation. A kink is created in the screw dislocation with edge character and length $|\mathbf{b}_E|$. If a stress is applied that moves the screw dislocation in its original slip plane, that same stress will cause the edge-character kink to move in the same slip plane. Therefore the kink does not make the dislocation (with the kink) sessile. However, if the screw components cross-slip to another slip plane, the kink will become a jog and make the dislocation sessile. We should this in recitation.



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.

Solution: Assume that 1 mm³ of well annealed metal contains about 10⁶ mm of dislocation per line length. In 1 mm³ of Al (FCC with a lattice parameter $a \simeq 4 \text{ \AA}$), there are

$$4 \text{ atoms} \times \left(\frac{10^{-3} \text{ m}}{4 \times 10^{-10} \text{ m}} \right)^3 = 6.3 \times 10^{19} \text{ atoms}$$

Next we must calculate the spacing between adjacent atoms on one edge dislocation. The closest spacing is $a/2 = 2 \text{ \AA}$. Therefore on 10⁶ mm of dislocation line there are

$$\frac{10^6 \text{ mm}}{2 \times 10^{-10} \text{ m/atom}} = 5 \times 10^{12} \text{ atoms}$$

The composition is therefore

$$\frac{5 \times 10^{12} \text{ solute atoms}}{6.3 \times 10^{19} \text{ total atoms}} = 10^{-7}$$

or 10⁻⁵%. Note that anything similar to this is acceptable.

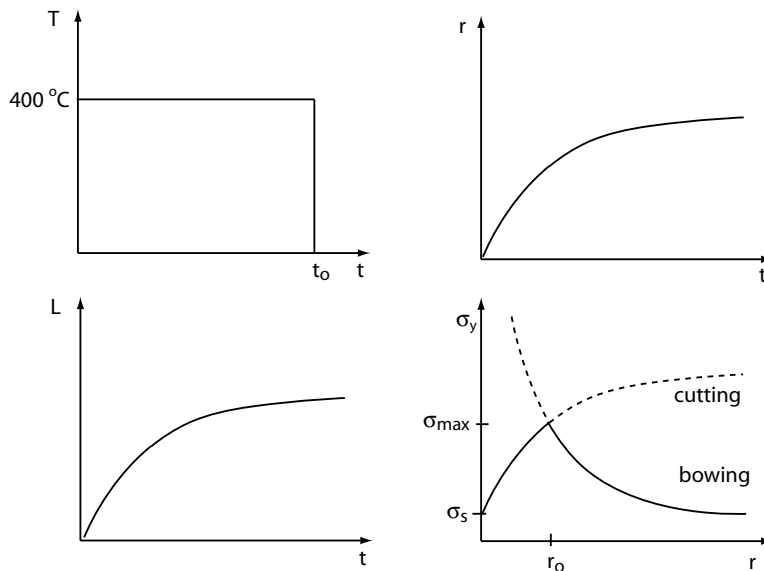
- (b) If you anneal the alloy at 400 °C, schematically show a plot of temperature vs. time, particle size r vs. time, particle spacing L vs. time, and yield strength vs. particle size. (Treat any additional equilibrium phases in a continuum manner ignoring interfaces and atomic structure.) In the last plot, describe the different strengthening mechanisms, including relative magnitudes, the would be the effective mechanisms at different times.

Solution: The first thing we have to realize is that the Al-Cu phase diagram tells us that at 2 at.% Cu and 400 °C, the equilibrium phases are Al and Al₂Cu. Therefore,

when we heat the sample to 400 °C, the Cu will precipitate out of solution to form Al₂Cu.

The figure below are the four plots (schematically) requested for this problem. The particle size r -time t plot assumes diffusion limit growth, therefore I assumed that r goes as $t^{1/2}$. Because the volume fraction of Cu is constant, as the particles grow (by coalescence) the spacing between the particles L must also increase with time; and will do so at a rate similar to the change of r with t .

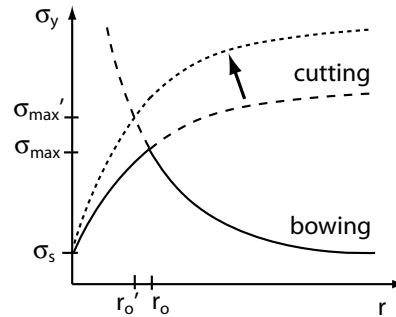
The yield strength resulting from this precipitation is shown schematically in the last plot. Because Cu is a substitutional solute in Al, the yield strength of the solid solution Al-Cu will only be slightly higher than the yield strength of pure Al. As precipitation begins and r increases, the dislocations will have to either cut through or bow around the precipitates. We noted in class and recitation that in the case of cutting, the strength of the material goes as $r^{1/2}$, and that for bowing it goes as L^{-1} , which is related to r^{-1} as noted above. Plotting these two curves schematically we note that they cross at a critical precipitate size r_o . At this point is where the maximum yield strength is observed. At $r < r_o$ it will be easier for dislocations to cut through the precipitates. At $r > r_o$ however, bowing is preferred.



- (c) Suppose instead of an alloy, you started with a composite of Al with Al₂O₃ 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.

Solution: The Al₂O₃ particles are stiffer (have a larger shear modulus G) than the

Al₂Cu precipitates. Thus for the same particle size, the line tension ($= Gb^2/2$) of a dislocation in an Al₂O₃ particle will be larger than that in an Al₂Cu precipitate. This implies a shift upwards of the cutting curve (see figure below). Therefore using Al₂O₃ particles instead of precipitation hardening, we can achieve a higher maximum yield strength (τ'_{\max}), but we must note that it occurs at a smaller radius (r'_o).



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.