

updated March 24, 2023

Contents

1 316-1 Problems

1

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Introduction

1) Send an email to Prof. Shull (k-shull@northwestern.edu) and Kyoungdoc (kyoungdockim2013@u.northwestern.edu) with the following information:

1. Anything about yourself (why you are interested in MSE, previous work experience, etc., outside interests apart from MSE) that will help me get to know you a bit (feel free to be brief - any info here is fine).
2. Your level of experience and comfort level with MATLAB. Be honest about your assessment (love it, hate it, don't understand it, etc.).
3. Let us know if you have NOT taken 314 or 315 for some reason.

Diffusion

2) Consider a diffusion couple with composition C_1 as $z \rightarrow -\infty$ and C_2 as $z \rightarrow \infty$. The solution to the diffusion equation is:

$$C(z, t) = \frac{C_1 + C_2}{2} - \frac{C_1 - C_2}{2} \operatorname{erf}\left(\frac{z}{2\sqrt{Dt}}\right)$$

where $\operatorname{erf}(y) = \frac{2}{\pi} \int_0^y e^{-t^2} dt$. Note that in the definition of the error function t is a dummy variable of integration, thus the error function is a function of y . Also, $\operatorname{erf}(0)=0$, and $\operatorname{erf}(\infty)=1$. You will determine if these boundary conditions are correct.

1. Show that the boundary conditions at $z = \pm\infty$ are satisfied by the solution.
2. Does the composition at $z = 0$ vary with time? If not, what is its value? Why do you think this is the case?
3. Write the solution in terms of $\eta = z/t^{1/2}$.
4. Show that the solution satisfies the following diffusion equation that is written in terms of η :

$$D \frac{d^2 C}{d\eta^2} + \frac{\eta}{2} \frac{dC}{d\eta} = 0$$

You will need to take a derivative of the error function. Leibniz's formula for the differentiation of integrals will be helpful:

$$\frac{d}{dz} \int_{h(z)}^{g(z)} f(t) dt = \frac{dg(z)}{dz} f(g(z)) - \frac{dh(z)}{dz} f(h(z))$$

3) A diffusion couple including inert wires was made by plating pure copper on to a block of α -brass with $X_{Zn} = 0.3$, as shown in Figure 1. After 56 days at 785°C the marker velocity was 2.6×10^{-8} mm/s, with a composition at the markers of $X_{Zn} = 0.22$, and a composition gradient, $\partial X_{Zn}/\partial z$ of 0.089 mm^{-1} . A detailed analysis of the data gives $\bar{D} = 4.5 \times 10^{-13} \text{ m}^2/\text{s}$ for $X_{Zn} = 0.22$. Use these data to calculate D_{Zn} and D_{Cu} for $X_{Zn} = 0.22$. How would you expect D_{Zn} , D_{Cu} and \bar{D} to vary as a function of composition?

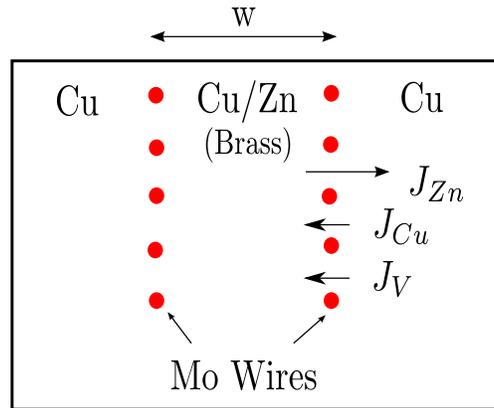


Figure 1: Experimental Geometry for the Kirkendall experiment.

4) In class we developed an expressions for J'_a . Show that $J'_a = -J'_b$. (Recall that these primed fluxes correspond to fluxes in the laboratory frame of reference).

5) Consider two binary alloys with compositions $X_b = X_1$ and $X_b = X_2$, shown in Figure 2 along with the free energy curves for α and β phases formed by this alloy. Draw the composition profile across the interface shortly after the two alloys are brought into contact with one another, assuming that the interface is in "local equilibrium", i.e. the interface compositions are given by the equilibrium phase diagram. Describe the direction in which you expect the B atoms to diffuse on each side of the interface.

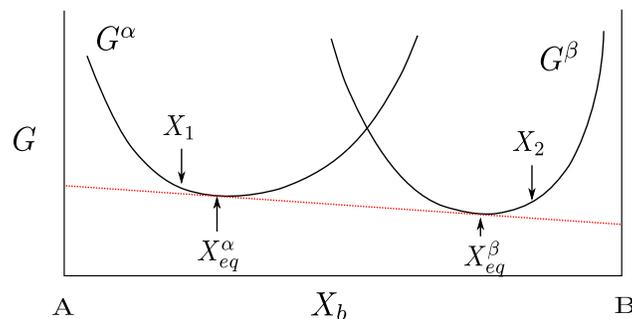


Figure 2: Free energy curves for a model A/B alloy.

6) The following MATLAB script runs the vacancy simulation shown in class. It saves the data into a 'structure' called output, which can be loaded into MATLAB later. The file can be downloaded from this link:

<http://msecure.northwestern.edu/316-1/matlab/vacancydiffusion.m>

```

1 tic % start a time so that we can see how long the program takes to run
2 n=30; % set the number of boxes across the square grid
3 vfrac=0.01; % vacancy fraction
4 matrix=ones(n);
5 map=[1,1,1;1,0,0;0,0,1]; % define 3 colors: white, red, blue
6 figure
7 colormap(map) % set the mapping of values in 'matrix' to a specific color
8 caxis([0 2]) % range of values in matrix goes from 0 (vacancy) to 2
9 % the previous three commands set things up so a 0 will be white, a 1 will
10 % be red and a 2 will be blue
11 matrix(:,n/2+1:n)=2; % set the right half of the matrix to 'blue'
12 i=round(n/2); % put one vacancy in the middle
13 j=round(n/2);
14 matrix(i,j)=0;
15 imagesc(matrix); % this is the command that takes the matrix and turns it into a
    plot
16 t=0;
17 times=[1e4,2e4,5e4,1e5];
18 showallimages=1; % set to zero if you want to speed things up by not showing
    images, set to 1 if you want to show all the images during the simulation
19
20 %% now we start to move things around
21 vacancydiff.matrices={}; % make a blank cell array
22 while t<max(times)
23     t=t+1;
24     dir=randi([1 4], 1, 1);
25     if dir==1
26         in=i+1;
27         jn=j;
28         if in==n+1; in=1; end
29     elseif dir==2
30         in=i-1;
31         jn=j;
32         if in==0; in=n; end
33     elseif dir==3
34         in=i;
35         jn=j+1;
36         if jn>n; jn=n; end
37     elseif dir==4
38         in=i;
39         jn=j-1;
40         if jn==0; jn=1; end
41     end
42     % now we need to make switch
43     neighborix=sub2ind([n n],in,jn);
44     vacix=sub2ind([n n],i,j);
45     matrix([vacix neighborix])=matrix([neighborix vacix]);
46     if showallimages
47         imagesc(matrix);
48         drawnow
49     end
50     if ismember(t,times)
51         vacancydiff.matrices=[vacancydiff.matrices {matrix}]; % append matrix to

```

```

        output file
52     imagesc(matrix);
53     set(gcf,'paperposition',[0 0 5 5])
54     set(gcf,'papersize',[5 5])
55     print(gcf,['vacdiff' num2str(t) '.eps'],'-depsc2')
56     end
57     i=in;
58     j=jn;
59 end
60 vacancydiff.times=times;
61 vacancydiff.n=n;
62 save('vacancydiff.mat','vacancydiff') % writes the vacancydiff structure to a .
    mat file that we can read in later
63 toc

```

1. Run the vacancy diffusion script, and include in your homework the .jpg files generated for time steps of $1e4$, $2e4$, $4e4$ and $1e5$.
2. For the longest time step, develop a plot of average composition along the horizontal direction.

Here is the MATLAB script that I used to do this (available at <http://msecore.northwestern.edu/316-1/matlab/vacancyplot.m>):

```

1 load vacancydiff % load the previously saved output.mat file
2 figure
3 figformat % not necessary, this is the standard initialization script I use
    to standardize what my plots look like
4 n=vacancydiff.n;
5 matrix=vacancydiff.matrices{4};
6 matrixsum=sum(matrix,1); % sum of each column in the matrix
7 plot(1:n,matrixsum/n,'+b')
8 xlabel ('z')
9 ylabel ('C')
10 print(gcf,'../figures/vacancyplot.eps','-depsc2') % this creates an .eps
    file, which I use for the coursenotes but which may not be as useful for
    many of you as the jpg file
11 % saveas(gcf,'vacancyplot.jpg') % this is what to do if you just want to
    save a .jpg file

```

Note that 'figformat' is NOT a matlab command. This line calls another file called names figformat.m that includes a few commands to standardize plots that I am making for this class. Here's what it looks like:

```

1 set(0,'defaultaxesbox','on') % draw the axes box (including the top and
    right axes)
2 set(0,'defaultlinelinerwidth',2)
3 set(0,'defaultaxesfontsize',16)
4 set(0,'defaultfigurepaperposition',[0,0,7,5])
5 set(0,'defaultfigurepapersize',[7,5])

```

3. In the previous problem set we obtained concentration profiles from the MATLAB. Now we'll take these concentration profiles and see if they are consistent with the solution to the diffusion equation.

- (a) For each of the 4 time points used in the simulation, plot the concentration profile and fit it to the error function to the diffusion equation, using the interfacial width, w , ($w = 2\sqrt{Dt}$) as a fitting parameter:

$$C(z, t) = \frac{C_1 + C_2}{2} - \frac{C_1 - C_2}{2} \operatorname{erf}\left(\frac{z}{w}\right)$$

Note: This problem is a curve fitting exercise in MATLAB. The most frustrating part is getting all the syntax right, but once you know the proper format for the MATLAB code, it's pretty straightforward. Take a look at the section entitled 'Fitting a Function to a Data Set' in the MSE MATLAB help file:

<http://msecore.northwestern.edu/matlab.pdf>

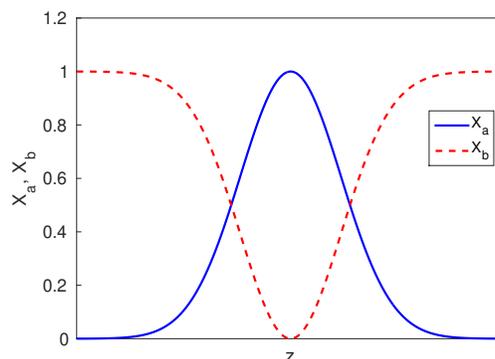
This section includes a MATLAB script that you can download and modify as needed.

- (b) Plot w^2 as a function of the time (expressed here as the number of time steps in the simulation). Obtain the slope of a line drawn through the origin that best fits the data.
- (c) When diffusion occurs by a vacancy hopping mechanism in a 2-dimensional system like the one used in our simulation, the diffusion coefficient is given by the following expression:

$$D = KX_v\Gamma a^2$$

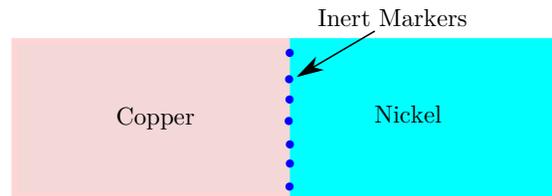
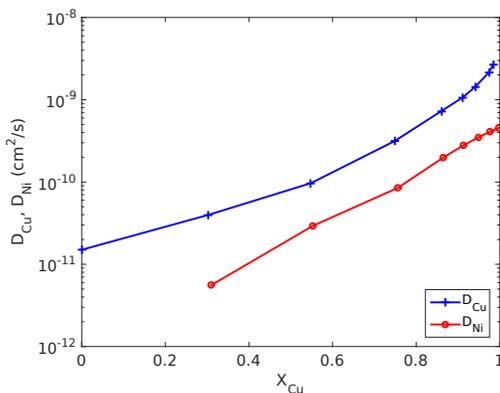
Here is the average hop frequency for any given vacancy and a is the hopping distance. From the the slope of the curve of w vs. the total number of jumps, extract an estimated value for K .

- 7) A region of material with a different composition is created in an infinitely long bar. The following plot shows the mole fraction of component A as a function of position. Assume that the intrinsic diffusion coefficient of the A atoms is twice as large as the intrinsic diffusion coefficient for the B atoms.

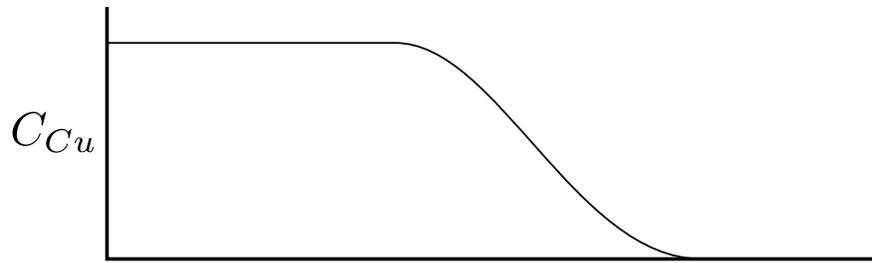


1. Plot the flux of A and the flux of B relative to the lattice as a function of position in the graph above.
2. Plot the vacancy creation rate as a function of position in the graph above.
3. Plot the flux of A and B in the lab frame as a function of position in the graph above.
4. Plot the lattice velocity as a function of position in the graph below. What are the physical implications of this plot?

8) The values for the intrinsic diffusion coefficients for Cu and Ni in a binary Cu/Ni alloy are shown below on the left (note that Cu and Ni are completely miscible in the solid state). A diffusion couple is made with the geometry shown below on the right.

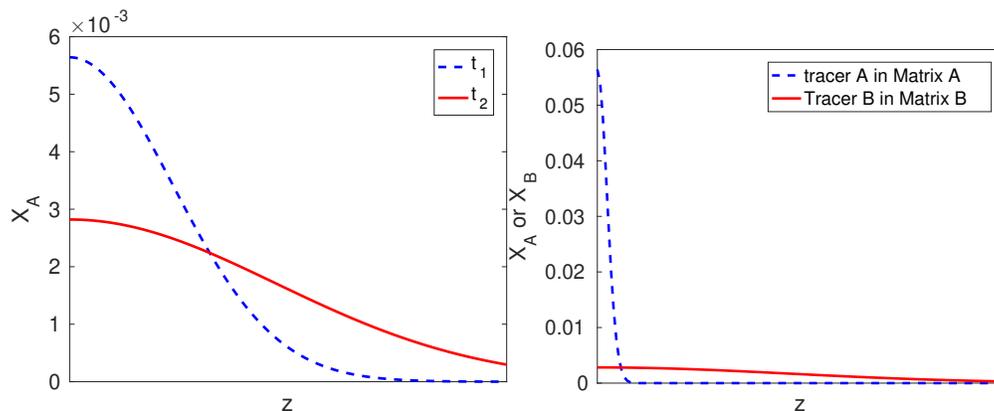


1. What is the value of the interdiffusion coefficient \tilde{D} , for an alloy consisting of nearly pure Nickel?
2. Will the markers placed initially at the Cu/Ni interface move toward the copper end of the sample, the nickel end of the sample, or stay at exactly the same location during the diffusion experiment.
3. The copper concentration across the sample is sketched below after diffusion has occurred for some time.

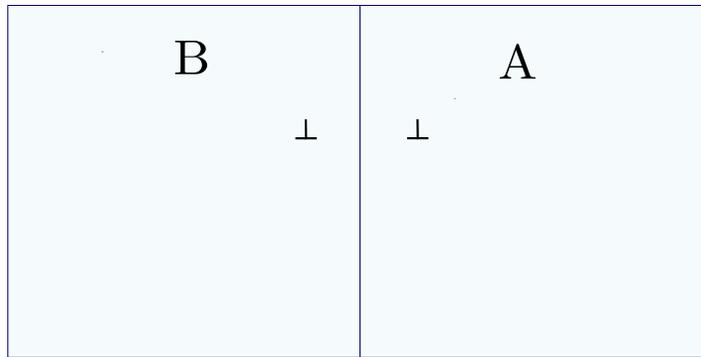


4. Sketch the fluxes of Copper, Nickel and vacancies, defining positive fluxes as those moving to the right.
5. Now sketch the rate at which vacancies are created or destroyed within the sample in order to maintain a constant overall vacancy concentration throughout.

9) An experiment is performed to determine the tracer diffusion coefficient of metal A in a matrix of metal B. This is done by depositing a very thin film of metal A onto the surface of metal B and measuring the concentration profile of metal A into the depth of the material at different times. The concentration profiles in the left figure below are obtained at two times, t_1 and t_2 :



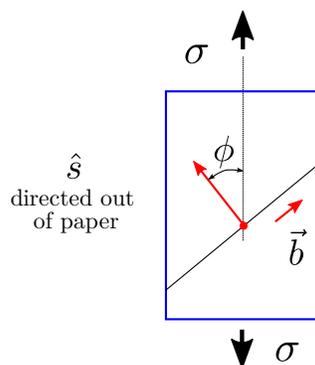
1. Estimate the ratio t_2/t_1
2. Now suppose we measure the self diffusion coefficients of A and B. Performing measurements at the same time and temperature gives the concentration profiles shown in the figure above to the right. Which element (A or B) do you expect has the highest melting temperature, and why?
3. Now we'll make a diffusion couple with element A on the right half and element B on the left half. Assume that A and B are miscible at the diffusion temperature, and form a one phase alloy. Mark up the following diagram as directed on the next page:



- Put an arrow labeled 'M' on the diagram indicating the direction that inert markers placed originally at the interface will move.
- Put an arrow labeled 'V' on the diagram indicating the the net vacancy flux due to diffusion in the sample.
- Put a 'C' on the region of the sample where you expect vacancies to be created, and a 'D' on the sample where you expect vacancies to be destroyed, assuming that the total vacancy concentration must remain at equilibrium.
- Two edge dislocations are also indicated in the diagram. Place arrows on top of each dislocation to illustrate he directions you expect these dislocations to move in order to create or destroy the vacancies from part iii.

Stress and Strain

10) A tensile stress, σ , is applied to a single crystal of zinc, which has an HCP structure. The close packed planes of atoms (the slip plane for an HCP material) is oriented with its surface normal in the plane of the paper, inclined to the tensile axis by an angle ϕ as shown below, with $\phi = 30^\circ$. Assume that the critical resolved shear stress for motion of the dislocation is 50 MPa (5×10^7 Pa). The shear modulus of Zn is 43 GPa (4.3×10^{10} Pa) and its atomic radius is 0.13 nm.

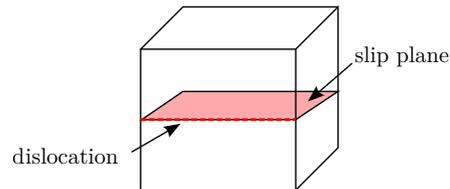


- Is this an edge dislocation, a screw dislocation, or a mixed dislocation, and how do you know?
- Put an arrow on the drawing above to indicate the direction in which the dislocation moves under an applied tensile stress.
- Calculate the tensile yield stress for this sample.

4. Suppose that the slip plane is oriented so that \vec{b} is still in the plane of the paper, but that ϕ is increased to 60° . Will the yield stress increase, decrease or stay the same.
5. Suppose that the dislocation is impeded by pinning points (precipitates, for example), that are uniformly spaced and separated by $1 \mu\text{m}$ (10^{-6} m). The resolved shear stress is determined by the stress required to move the dislocation around these pinning points. Use the information given in this problem to determine the energy per length of the dislocation. Compare this to the expressions given for the energies of edge and screw dislocations to see if it makes sense.

Dislocation Structure

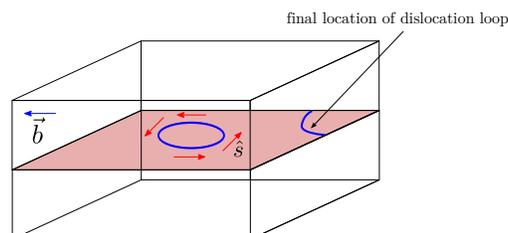
11) A right handed screw dislocation initially located in the middle of the front face of the sample shown below moves toward the back of the sample in response to an applied shear stress on the sample.



1. Sketch the shape of the sample after the dislocation has propagated halfway through the sample, and again when it has propagated all the way through the sample. Use arrows to specify the shear force that is being applied.
 2. Repeat part a for a left-handed screw dislocation.
- 12) Draw an edge dislocation and on the same figure dot in the positions of the atoms after the dislocation has shifted by \vec{b} .

13) How can two edge dislocations with opposite Burgers vectors meet to form a row of vacancies? How can they meet to form a row of interstitials? Draw pictures of both situations.

14) Given a crystal containing a dislocation loop as shown in the following figure:



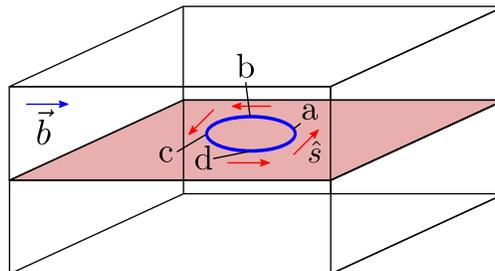
Let the loop be moved (at constant radius) toward a corner until three-fourths of the loop runs out of the crystal. This leaves a loop segment that goes in one face and comes out the orthogonal face. Sketch the resultant shape of the crystal, both above and below the slip plane.

15) Given a loop with a Burger's vector that is perpendicular everywhere to the dislocation line, determine the resulting surface morphology after the loop propagates out of the crystal. Assume that the loop moves only by glide.

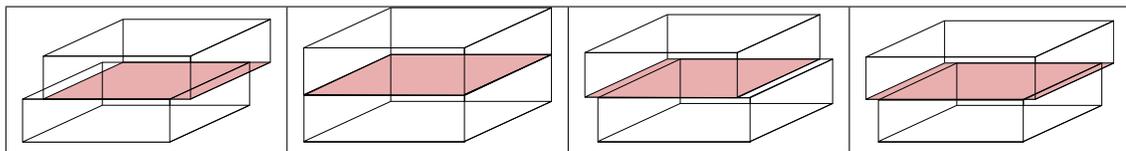
16) Show that it is impossible to make a dislocation loop all of whose segments are pure screw dislocations, but that it is possible with edge dislocations. For the case of the pure edge dislocation loop, describe the orientation of the extra half plane with respect to the dislocation loop.

17) Draw the compressive and tensile regions surrounding an edge dislocation.

18) Consider the dislocation loop shown below:



1. Circle the drawing below that corresponds to the shape of the material after the dislocation has expanded and moved out outside the crystal.



2. Indicate in the spaces below the locations (a, b, c, or d) where the dislocation has the following characteristics:

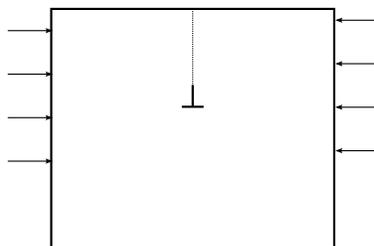
(a) It is a right handed screw dislocation: _____

(b) It is a left handed screw dislocation: _____

- (c) It is an edge dislocation with the extra half plane above the plane of the loop: _____
- (d) It is an edge dislocation with the extra half plane below the plane of the loop: _____
3. Add arrows to the illustration of the dislocation loop to show the orientation of the shear stress that will most efficiently cause the dislocation to loop to grow.

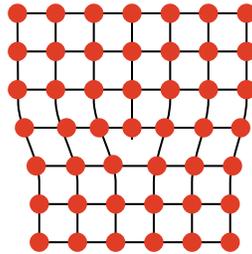
Dislocation Interactions

- 19) If edge dislocations with opposite signs of the Burger's vectors meet, does the energy of the crystal increase or decrease? Defend your answer.
- 20) A nanowire is grown such that it is free of dislocations. Why would the stress required to deform the nanowire be larger than a bulk material?
- 21) If an anisotropic alloy system has a nearly zero dislocation line tension, would you expect the precipitate spacing to have a large effect on the yield stress of the alloy? Explain your reasoning
- 22) Given an edge dislocation in a crystal, whose top two-thirds is under a compressive stress σ acting along the glide plane (see figure below):

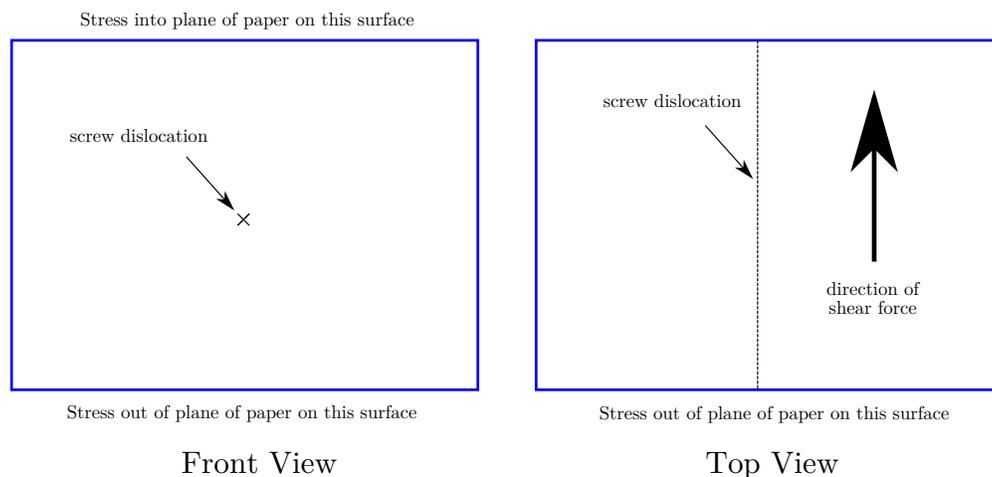


1. If diffusion occurs, which way will the dislocation move? Explain why and tell where the atoms go that leave the dislocation.
2. Derive an equation relating the stress, σ to b and the force tending to make the dislocation move in the vertical plane.
3. If the edge dislocation is replaced by a screw dislocation, which way will the dislocation tend to move?

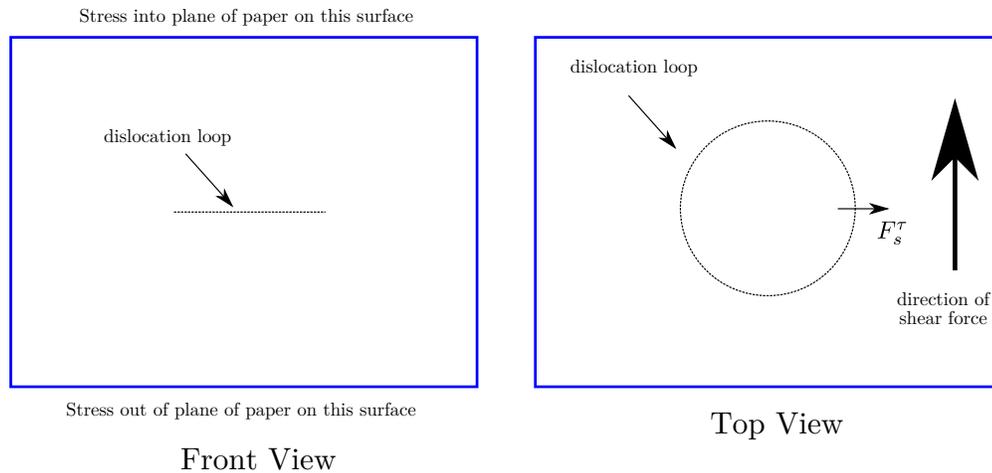
- 23) Construct a plot of the interaction energy vs. dislocation separation distance for two identical parallel edge dislocations that continue to lie one above the other as climb occurs. Justify your plot qualitatively by explaining how the strain energy changes with vertical separation.
- 24) Repeat the previous problem for edge dislocations of opposite sign.
- 25) On the following sketch of a dislocation, indicate the direction that it must move in order for vacancies to be created.



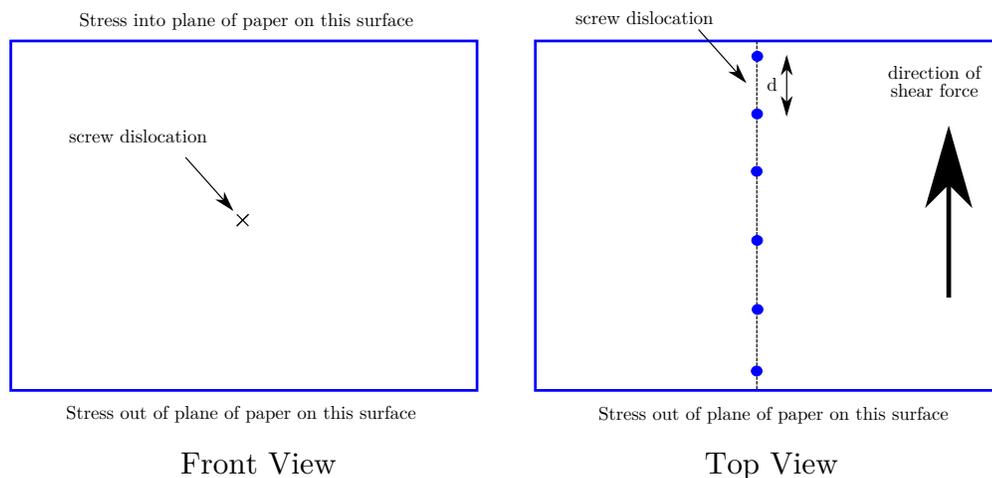
- 26) Consider an isolated right-handed screw dislocation. Suppose a shear force is applied parallel to the dislocation line, as illustrated below.



1. What is the direction of the force, F_s^T , that is applied to the dislocation as a result of the applied stress.
2. Suppose the screw dislocation is replaced by a dislocation loop with the same Burgers vector as the dislocation from part a, as shown below. Use arrows to indicate the direction F_s^T at different points along the dislocation loop. (The direction of F_s^T has already been indicated at the right edge of the dislocation).



3. Describe how the magnitude of F_s^τ changes (if at all) for different locations along the dislocation loop.
4. What do you expect to happen to the dislocation loop if you remove the external applied stress (will the loop grow, shrink or stay the same size)?
5. Suppose the straight screw dislocation from is pinned by obstacles that are separated by a distance d , as illustrated in the following figure. Sketch the shape of the dislocation for an applied shear stress that is just large enough for dislocation to pass around the obstacles.



6. What do you expect to happen to the critical resolved shear stress of the material if d is decreased by a factor of 2. (Will the critical resolved shear stress increase, decrease or stay the same).

Interfacial Thermodynamics

27) Consider the following:

1. Is the molar latent heat positive or negative?
2. Is the melting temperature, T , for a very small particle greater to or less than the equilibrium value of T_m for a bulk material?
3. Must this always be the case?
4. For metals, what is the typical value of r for which a change in melting temperature of 10K is observed. What about a change of 1K?

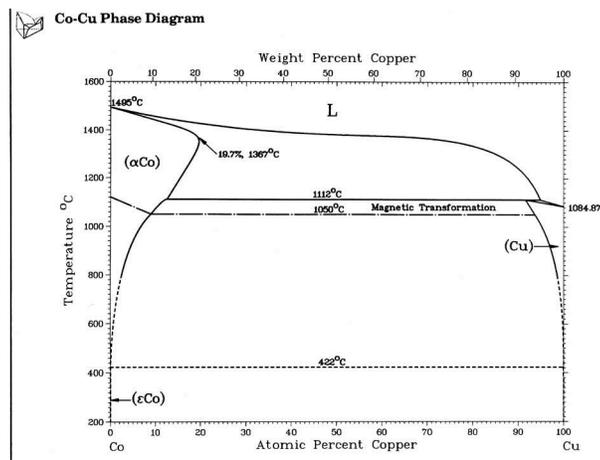
28) The molar enthalpy of a phase varies with temperature as

$$H_m(T) - H_m(T_0) + \int_{T_0}^T C_p(T) dT$$

where C_p is the molar heat capacity. Given this, at what temperature is the latent heat appearing in expression for the melting point reduction evaluated?

29) Consider the case of a pure liquid spherical droplet embedded in a pure solid. Create a graphical construction plotting the temperature dependence of the free energy of the solid and liquid phases for this case, and use it to determine if the melting point above or below the bulk melting temperature.

30) Consider the Co-Cu phase diagram shown below:



1. Plot the equilibrium activity of Cobalt as a function of composition across the entire phase diagram at 900°C.

- From the phase diagram, estimate the solubility limit of Co in Cu at 900 °C. Suppose the interfacial free energy for the Cu/Co interface is 300 mJ/m². For what radius of a Co precipitate will this solubility limit be increased by 10%?

Surface and Interface Structure

31) Look up values for heats of sublimation for any of the materials in Table 6.1 that have close-packed crystal structures (FCC or HCP). Compare the estimated values of the surface free energy that you obtain from these heats of sublimation to the tabulated values in Table 6.1.

32) Determine the equilibrium shape of a crystal. This should be done using a computer and your favorite program or language (most likely MATLAB). The equation of a straight line in polar coordinates drawn from the origin of the polar coordinate system is $r \cos(\theta - \alpha) = d$, where (r, θ) locate the points on the line, d is the perpendicular distance from the origin to the line and α is the angle between the perpendicular to the line and the x-axis (see Figure3).

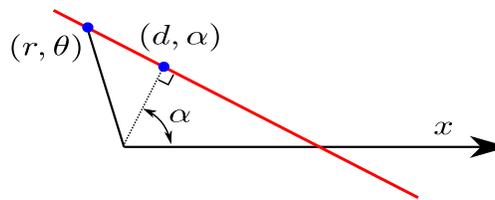


Figure 3: Representation of a line drawn a distance d from the origin.

- Determine the equilibrium shape of a crystal where the surface energy is given by $\gamma = 1$ J/m² (independent of α).
- Determine the equilibrium shape of a crystal where the surface energy is given by $\gamma = 1 + 0.05 \cos(4\alpha)$ J/m² (α in radians). Are there any corners on the equilibrium shape?
- Determine the equilibrium shape of a crystal where the surface energy is given by $\gamma = 1 + 0.07 \cos(4\alpha)$ J/m². Are there any corners on the equilibrium shape?
- Determine the equilibrium shape of a crystal where the surface energy is given by $\gamma = 1 + 0.6 \cos(4\alpha)$ J/m². Are there any corners on the equilibrium shape? How is the shape shown in (c) different from that in (d), and why (argue on the basis of the physics of the problem)?

As a headstart on this problem, here's a MATLAB script that generates polar plots of the γ as defined in the problem:

```

1 close all
2 A=[0,0.05,0.07,0.6]; % these are the 4 values of A defined in the problem
3 % define a function where the radius d is the surface energy and alpha
4 % is the angle
5 d=@(A,alpha) 1+A*cos(4*alpha);
6 figure

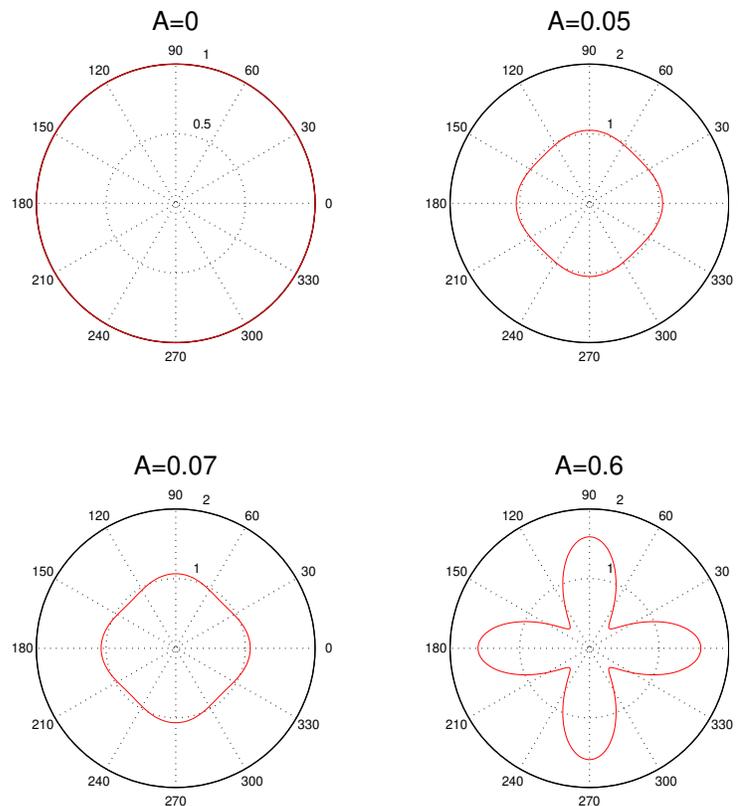
```

```

7 for k=1:4
8     alpha=linspace(0,2*pi,200);
9     subplot(2,2,k) % this makes a 2 by 2 grid of plots
10    polar(alpha,d(A(k),alpha),'r-'); % polar is the command to make a
    polar plot
11    title(['A=' num2str(A(k))],'fontsize',20) % label each subplot
12 end
13 % adjust the print command as necessary to change the format, filename,
14 % etc.
15 print(gcf,'../figures/matlabwulffenergy.eps','-depsc2') % save the eps
    file

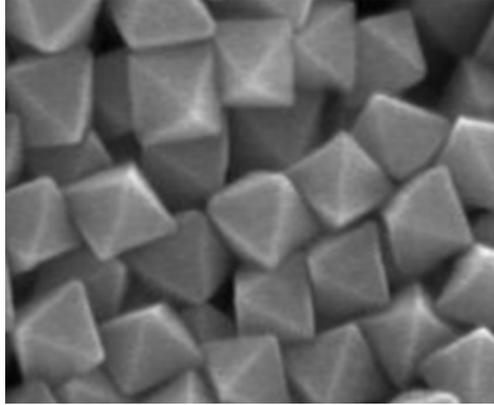
```

This generates the following polar plots for the four different functions that are given (with A defined so that $\gamma = 1 + A \cos(4\alpha)$).



33) Assume a simple cubic crystal structure with nearest neighbor interactions. Calculate the ratio of the surface energies for the $\{110\}$ and $\{100\}$ surfaces.

34) The octahedral particles of FCC golds shown below were created by controlling the growth rates of the different crystal facets. For these crystals, were the growth rates fastest in the $\langle 100 \rangle$ directions or in the $\langle 111 \rangle$ directions? Provide a brief explanation of your answer.



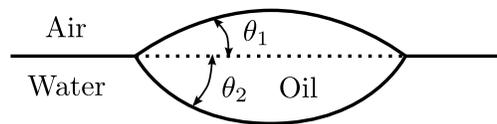
35) The relationship between the the interfacial energy between α and β phases and the pressure difference across a curved interface is obtained from the following expression:

$$-P^\alpha \delta V^\alpha - P^\beta \delta V^\beta + \gamma_{\alpha\beta} \delta A^\Sigma = 0$$

1. Use this expression to obtain the pressure difference between a cylinder of β phase with a radius r and a surrounding α phase.
2. Repeat the calculation for a cube where the length of each side is a . Assume that the surface energy of each of the cube faces is the same.

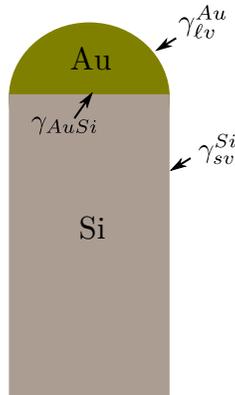
Wetting and Contact Angles

36) Consider the an oil droplet that forms on the surface of water, as shown schematically in the following Figure:



Determine θ_1 and θ_2 if the air/water interfacial free energy is 72 mJ/m^2 , the air/oil interfacial free energy is 30 mJ/m^2 and the oil/water interfacial free energy is 50 mJ/m^2 .

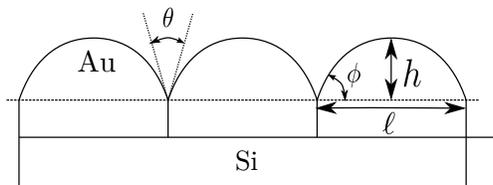
37) Suppose a, hemispherical liquid Au droplet with a radius of curvature of r is in contact with solid Si cylinder with the same radius as shown below. Derive a relationship between the three interfacial energies that must be valid in order for the equilibrium shape of the Au/Si interface to be flat, as drawn in the picture.



Grain Boundaries

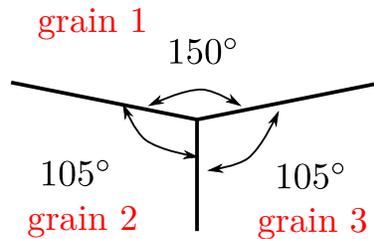
38) The surface energy of the interface between nickel and its vapor is 1.580 J/m^2 at 1100K . The average dihedral angle measured for grain boundaries intersecting the free surface is 168° . Thoria dispersed nickel alloys are made by dispersing fine particles of ThO_2 in nickel powder and consolidating the aggregate. The particles are left at the grain boundaries in the nickel matrix. Prolonged heating at elevated temperatures gives the particles their equilibrium shape. The average dihedral angle measured inside the particle is 145° . Estimate the interfacial energy of the thoria-nickel interface. Assume the interfacial energies are isotropic.

39) Consider a gold line deposited on a silicon substrate. The grain boundaries run laterally completely across the line, giving a "bamboo" structure as shown in the figure below. The grain boundary energy of gold at 600K is 0.42 J/m^2 and the surface energy is 1.44 J/m^2 . Assume all the interfacial energies are isotropic.

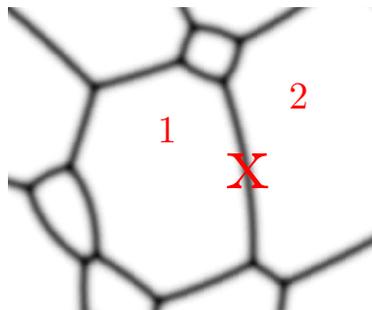


1. Compute the dihedral angle (θ in the diagram above) where a grain boundary meets the external surface.
 2. Find the critical grain boundary spacing ℓ_c for which the equilibrium grain shape produces a hole in the film, assuming $h = 1 \mu\text{m}$. Note that for a spherical cap, ℓ , h and ϕ are related to each other by the following expression: $\tan(\phi/2) = 2h/\ell$.
- 40) Why does the velocity of a grain boundary depend on temperature? Assume that the driving force for grain boundary motion is independent of temperature.

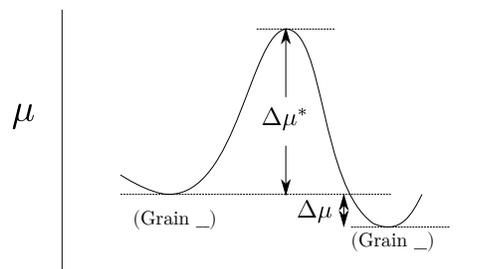
- 41) Consider the following junction between three grains. Suppose that the grain boundary free energy between grains 1 and 2, and between 1 and 3, is 0.5 J/m^2 . What is the grain boundary energy between grains 2 and 3?



- 42) Consider the following image from the grain growth simulation:



- The boundary marked with an 'X' separates grains 1 and 2. Do you expect this boundary to move toward grain 1 or grain 2 during the process of grain growth?
- Suppose that the interface marked above is the cross section through a grain boundary in aluminum, and that this section of the grain boundary has a spherical shape with a radius of curvature of $1 \mu\text{m}$. Assuming a grain boundary energy of 0.25 J/m^2 , calculate the chemical potential difference, $\Delta\mu$ between Al atoms on the '1' and '2' sides of the grain boundary.
- On the schematic below, indicate which grain is grain 1 and which one is grain 2.



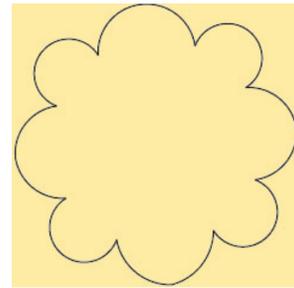
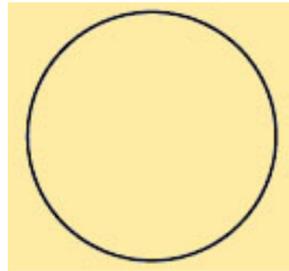
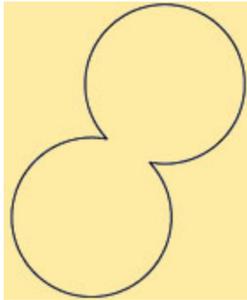
- Suppose $J_{1 \rightarrow 2}$ is the rate at which Al atoms hop from grain 1 to grain 2, and $J_{2 \rightarrow 1}$ is the rate at which atoms hop from grain 2 to grain 1. Calculate the ratio, $J_{1 \rightarrow 2} / J_{2 \rightarrow 1}$ at $T = 500\text{K}$.

Transformation Kinetics

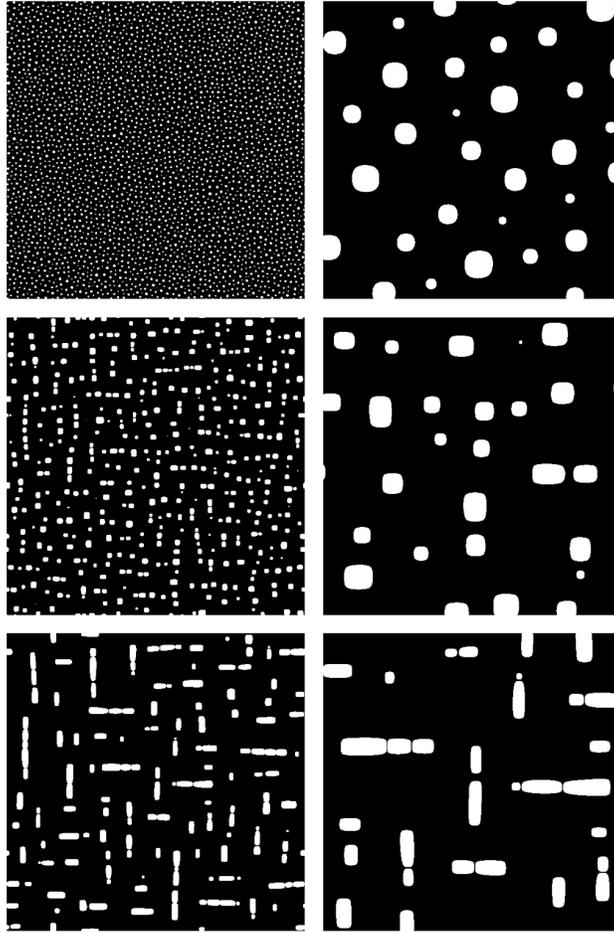
43) Does the time to 50% transformed increase or decrease with an increase in nucleation rate? Defend your answer without using any equations.

Interphase Interfaces

44) Consider a material with the orientational dependence of the surface energy shown in each of the 3 plots below. For each of these three materials, sketch the equilibrium shape that you would expect to obtain. On each drawing, indicate any interfaces that you expect to be coherent.



45) Consider the shapes of the particles in the simulations below of misfitting particles in an elastically anisotropic system. The left column is the entire system, whereas the right column is a magnification of a small region of the figure in the left column. These are snapshots taken as function of time while the particles are growing. Are these cuboidal shapes due to elastic stress, an anisotropic interfacial energy, or both?

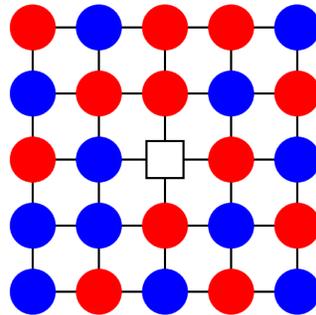


- 46) Explain the structure and energies of coherent, semicoherent and incoherent interfaces, paying particular attention to the role of orientation relationships and misfit.
- 47) Explain why fully coherent precipitates tend to lose coherency as they grow.
- 48) Why do very small precipitates tend to have coherent interfaces?
- 49) A thin film of Zn with an HCP crystal structure is deposited on a Ni FCC substrate with a {111} orientation. Which plane of the HCP crystal would you expect to contact the {111} Ni surface?
- 50) Given an example of an interface between two crystals that that displays a very large change in free energy with a change in the orientation of the interface.

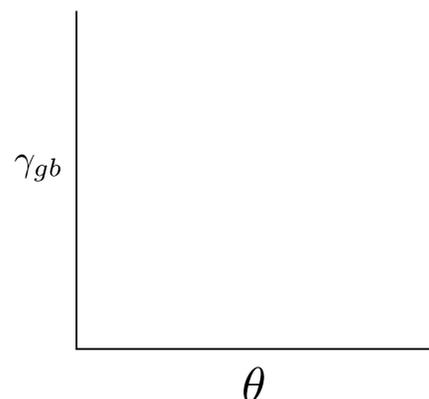
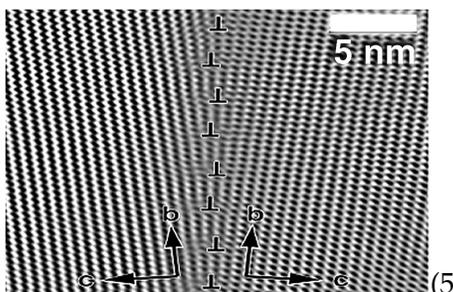
51) Consider an FCC metal (metal A) with a surface energy of 1 J/m^2 . An HCP metal (metal B) with a surface energy of 0.7 J/m^2 is deposited onto the $\{111\}$ surface of metal A. Assume that the atomic diameter of the HCP metal is 3% larger than the atomic diameter of the FCC metal, and that the chemical component of the interfacial energy between the two metals is 0.2 J/m^2 .

1. For B layers that are sufficiently thin, do you expect that a coherent interface will form between the A and B materials? Justify your answer.
2. How do you expect the interface between the A and B metals to change as the thickness of the B layer increases?
3. Do you expect thick films to remain continuous, or will isolated drops of B be formed on the surface. Describe any assumptions that you make.

52) Consider the vacancy shown below, for a simulation of 'red' and 'blue' atoms that are undergoing phase separation. Is the vacancy more likely to move to the right or to the left? Justify your answer.



53) Consider the tilt boundary shown in the image to the left. On the axes on the right, sketch the relationship between the grain boundary free energy and the tilt angle that you expect to observe for values of theta between 0 and 10° .



54) Suppose you need to apply a coating to a surface, and you want the coating to spread as a smooth uniform film for all thicknesses. You have a choice of three different coatings, which have the thickness-dependent free energies shown below. Which material to you choose, and why?

