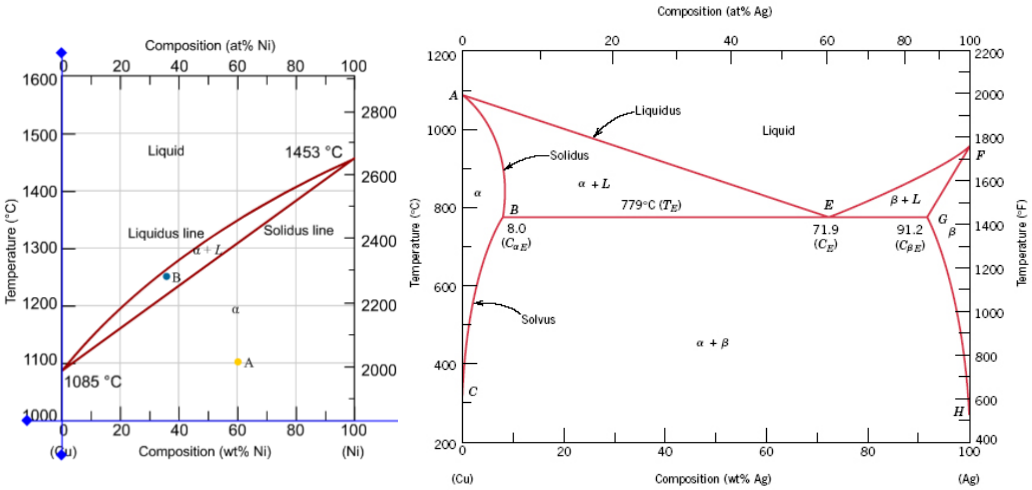
Homework 10

Exercise 1

Our goal in this exercise is to better understand binary phase diagrams and develop some intuition. Below are the Cu-Ni and Cu-Ag phase diagrams.



a. If the two components A, B of a binary phase diagram have a different crystal structure, is it possible that the binary phase diagram looks like the one on the left close to the ideal mixture model?

b. The elements Cu, Ni, Ag and Au and Al all have fcc crystal structures, with lattice parameters in Angstrom given in the table.

Ni	Cu	Ag	Au	Al
3.52	3.61	4.09	4.08	4.05

The Ni-Cu and Ag-Au systems have a phase diagram close to the one predicted by the ideal model shown on the left, while Cu-Ag has a eutectic phase diagram shown on the right. Based on just this information: what could influence whether a binary phase diagram is (close to) ideal?

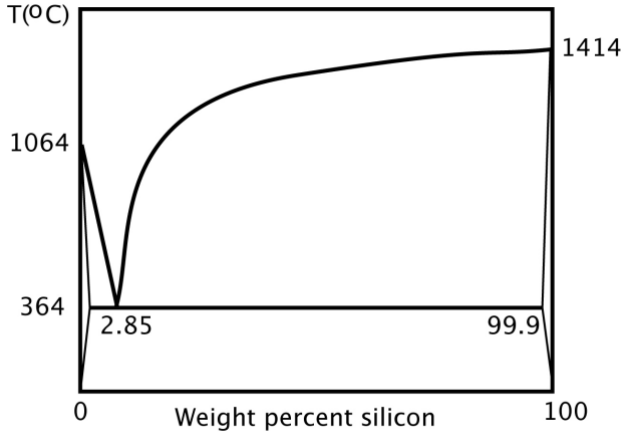
If we assume that the three systems mentioned above can be described by the regular solution model, would their interaction parameter Ω_{solid} be positive, close to zero, or negative? [you can assume that $\Omega_{liquid} = 0$] How can we intuitively understand those values of Ω_{solid} using the lattice parameters? Hint: Recall that Ω_{solid} represents the energetic cost of mixing.

c. Predict for which of the remaining combinations of elements in the table, the phase diagram will look close to ideal.

d. Experimentally, the Al-Ag and Al-Au phase diagrams are very complicated and far from the ideal mixture model. On top of having the same crystal structure and lattice constant, the components also need to have very close chemical behavior: similar electronegativities, bonding etc., to be miscible at all temperatures. How could this explain the difference in the Ag-Au and Ag-Al diagrams?

Exercise 2

Nanowires are explored as the functional component for next generation electronic devices. One possible way of growing silicon nanowires is to place gold nanoparticles of a given diameter (for example, 5 nm) on an inert surface and supply them with a supersaturated silicon vapor. A property of the supersaturated gas is that it continuously 'pushes' silicon onto the gold nanoparticles. In other words the gold particles start as pure gold but as time progresses, they become gold-silicon particles with an ever-increasing atomic fraction of silicon. In this problem we try to understand why this process leads to silicon nanowires. The phase diagram of gold and silicon is shown in the figure below. Notice that the x-axis is not linear as the extremes (i.e. the parts close to 0 and 1) are enlarged for the sake of visualization. Assume that the gold nanoparticles never change shape and size during the nanowire growth.



Starting from an initial state of pure gold, the nanowire growth is performed at 400°C.

a. Illustrate with a line on the diagram the evolution of the materials as time progresses.

b. Please explain when solid silicon will start forming and why.

c. Indicate on the phase diagram the composition and physical state (vapour, liquid, or solid) of the gold nanoparticles when silicon nanowires start to form.

d. When the silicon source is removed, the surface is allowed to cool down to room temperature. Describe the nanowire composition if the surface is cooled down slowly in an ideal equilibrium process.

e. In reality, when silicon is solid, very little mobility of gold is achieved. Therefore, as the wires are cooled down they do not change their composition (i.e. they stay in a kinetically trapped composition that matches the composition at 400°C). Given that for electronic applications, gold is an unwanted impurity, what is a better temperature for growing silicon nanowires, 400°C or 1000°C? Please explain your answer.

f. What is the maximum temperature at which this process still works?