

Using the Equal Gibbs method to generate re-entrant phase diagrams

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Background:

Re-entrance means that at a given composition solely by raising the temperature I can start out in a phase, transition to another phase then by continuing to raise the temperature transition back to the first phase. To model this we used the Equal Gibbs Curve method which is the following equation

$$(1-x)\Delta\mu^1(T) + x\Delta\mu^2(T) + \Delta G^E = 0$$

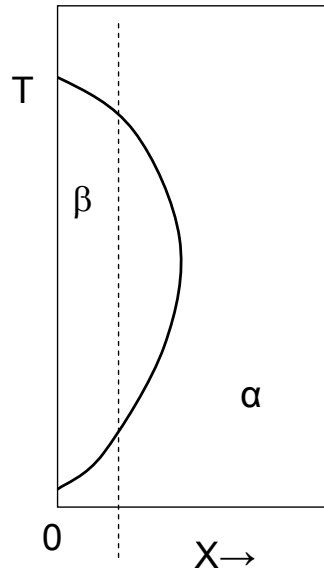
Approach:

The idea was to automate the drawing of the Equal Gibbs Curves such that they could be calculated quicker and easier. Once the drawing was automated I would then attempt to draw several Equal Gibbs curves and look for abnormalities.

Results: I automated the drawing of the Equal Gibbs Curves (EGC) by writing several Mathematica programs. Each program has its benefits and its downsides. The drawing of phase diagrams found a few possibilities for second order phase transition. When they found a few regions where the temperature had to have an imaginary component to solve the Equation defining the Equal Gibbs Curve

Future Work: To figure out if the imaginary regions are signifying second order phase transitions. Also use some experimental data and see how close the models predictions are.

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Research Experience for Undergraduates



A simple re-entrant system. You can see that as you travel along the dotted line you transition from alpha phase to beta phase and back again.

