ICMEd Summer School Thermo. Module

Summer 2017 Mason/Thornton/Aagesen

Computational Methods in MS&E

Computational Thermodynamics Module Problems

1. Following the walkthrough and using the TCBIN database, plot and print out (or capture its image if you will be using an electronic document) the Gibbs free energy versus composition for the Cu-Ni system at 1473 K using Thermo-Calc. For compositions in the approximate range of 0.25-0.30 mole fraction Ni, the system will phase separate to lower its free energy. Determine, via common-tangent construction (by hand on a printout or drawing lines on the figure within an electronic document), the equilibrium composition of each stable phase and report. Explain in your own words why the common tangent construction determines phase equilibrium in a plot of Gibbs free energy versus composition.

2. Calculating the phase diagram of an Al-Si alloy. Al-Si alloys are frequently used in castings due to their combination of good physical properties and excellent castability. In this exercise you will manually calculate several phase boundaries of the Al-Si binary phase diagram and compare to Thermo-Calc calculation.

a. Using Thermo-Calc with the database TCBIN, plot Gibbs free energy versus composition for each phase for the following temperatures: 820 K, 850 K, 888 K, 1273 K. (When you have generated the first plot, let an instructor know and they will check your plot and give you a printout of the plot for each temperature.) Following the same process as in #1, determine the stable phases at each temperature and mole fraction at the phase boundaries using the common tangent construction.

b. Plot the binary Al-Si phase diagram using Thermo-Calc with the database TCBIN. (When you have generated the first plot, let an instructor know and they will check your plot and give you a printout of the plot for each temperature.) On the printout, plot the mole fractions of the phase boundaries at each temperature you determined in part a. (Note: the default units on phase diagram plots are °C, please make sure to you change the axis to K.)

c. Using the database ALDEMO, plot the phase fraction of the stable phases as a function of mole fraction Si (*xSi*) in the range 0 to 0.1 at 773 K. Calculate the phase fraction of the stable phases at this temperature at *xSi* = 0.05 using only the Al-Si phase diagram. Also, plot the mole fraction of Si in the Al-rich FCC phase (FCC\_A1) for *xSi* in the range 0 to 0.1 at 773 K.

d. The addition of Magnesium to Al-Si alloys increases hardness due to the formation of Mg2Si precipitates. Using the database TCAL4, plot an isopleth of the Al-Si-Mg system for Si concentration of 5 mass %, for Mg concentration from 0 to 10 mass %. At 820 K, at what Mg concentration do Mg2Si precipitates first become thermodynamically stable? Please have an instructor check your plot and your answer before proceeding to the next question.

3. Martensitic stainless steels offer a combination of high mechanical strength and corrosion resistance. To increase the hardness of the surface, the process of “carburization”, or annealing in the presence of a carbon-rich gas, can be performed, which will increase the carbon concentration in the steel near the surface. However, the increase in hardness must be balanced against a loss of corrosion resistance. This exercise will help understand the reasons for this trade-off. The nominal composition of a particular industrial martensitic stainless steel is (by mass percent)

Cr 13

Co 5

Ni 3

Mo 2

C 0.07.

Fe balance (76.93, but leave this blank)

(Usually when specifying steel compositions this would be written Fe-13Cr-5Co-3Ni-2Mo-0.07C, where composition is written prior to each element, and the Fe composition is omitted since it is the main constituent.) Carburization causes an increase in carbon concentration near the surface, leading to the formation of chromium-rich carbide phases within the FCC matrix, including M23C6, M7C3, and M3C. (where M stands for metal). M23C6 and M7C3 increase hardness, but the formation of M3C (also called cementite) reduces strength.

a. Using Thermo-Calc with the database TCFE8, plot an isopleth of this steel for mass percent carbon varying from 0-10 mass-%, and plot the phase fractions as a function of mass percent carbon at 1230 K in the range 0-10 mass-% carbon.

b. Using the results of part (a), at a temperature of 1230 K, determine the range of mass percent carbon that allows M23C6 and/or M7C3 to form, but prevents cementite from forming (carburization will not raise C content dramatically which is why you can limit your search to <10 mass % C). Compare with the answer above.

c. Corrosion resistance in stainless steels is significantly enhanced by the presence of Cr in the FCC matrix phase. After carburization, it has been found that corrosion resistance at the surface decreases. Explain why this occurs using a plot of Cr content of the FCC phase versus carbon concentration.

**Alternate version of Problem 3:** This more simplified problem can be done with the public database FEDEMO, for institutions that do not have access to TCFE8.

Martensitic stainless steels offer a combination of high mechanical strength and corrosion resistance. To increase the hardness of the surface, the process of “carburization”, or annealing in the presence of a carbon-rich gas, can be performed, which will increase the carbon concentration in the steel near the surface. However, the increase in hardness must be balanced against a loss of corrosion resistance. This exercise will help understand the reasons for this trade-off. The most basic martensitic stainless steel is Type 410, which has a nominal composition of (by mass percent)

Cr 13.5

C 0.15.

Fe 86.35

(Usually when specifying steel compositions this would be written Fe-12.5Cr-0.15C, where composition is written prior to each element, and the Fe composition is omitted since it is the main constituent. 410 steels may also include a small amount of Mn which is primarily used to combine with and remove oxygen impurities; it can be neglected for the purposes of this exercise.) Carburization causes an increase in carbon concentration near the surface, leading to the formation of chromium-rich carbide phases within the FCC matrix, including M23C6, M7C3, and M3C (where M stands for metal). M23C6 and M7C3 increase hardness, but the formation of M3C (also called cementite) reduces strength.

a. Using Thermo-calc with the database FEDEMO, plot an isopleth of this steel for mass percent carbon varying from 0-5 mass-%, and plot the phase fractions as a function of mass percent carbon at 1230 K in the range 0-5 mass-% carbon.

b. Using the results of part (a), at a temperature of 1230 K, determine the range of mass percent carbon that allows M23C6 and/or M7C3 to form, but prevents cementite from forming (carburization will not raise C content dramatically which is why you can limit your search to <5 mass % C).

c. Corrosion resistance in stainless steels is significantly enhanced by the presence of Cr in the FCC matrix phase. After carburization, it has been found that corrosion resistance at the surface decreases. Explain why this occurs using a plot of Cr content of the FCC phase versus carbon concentration.