Homework 13 Advanced Thermodynamics
Due Tuesday November 24, 2020

Nanocrystalline materials can have exceptional mechanical properties compared to conventional crystals. The yield strength can increase following the Hall-Petch relationship $\sigma_y = \sigma_0 + Kd^{-1/2}$. Nanocrystalline materials do not strain harden so they display perfect or super-plasticity. The modulus decreases by 30 to 50%. Grain growth or coarsening of nanocrystalline metals during processing has hindered their application. Saber M; Kotan H; Koch CC; Scattergood RO *Thermodynamic stabilization of nanocrystalline binary alloys* J. Appl. Phys. **113** 063515 (2013) developed a predictive thermodynamic model for stabilization of nanocrystalline binary alloys using a regular solution model.

a) Explain the general features of an ideal solution and a regular solution model. Derive the entropy and enthalpy expressions for these models using a statistical thermodynamics approach.

b) Nanograin size can be explained by kinetic stabilization or by thermodynamic stabilization. Explain the logic behind these two models. What is the advantage of a metastable state model?

c) Weissmuller J *Alloy Effects in Nanostructures* Struc. Mat. B 261-272 (1993) in Figure 1 shows three possible scenarios for solid solutions involving grain boundaries. How does Saber et al. account for these three possibilities in their model?

d) Introduction of a solute atom in a lattice leads to lattice strain. This strain could be relieved if the solute were located at a grain boundary. In addition to this elastic component, there is a chemical advantage to locating the solute at a grain boundary. Explain the origin of the chemical advantage and how it is incorporated in Saber's model.

e) Derive Saber's equation 12.

f) "z" doesn't seem to be constant between the interface and the grains in Figure 1 of Saber. Explain how this is accounted for in Saber's model.

g) Weissmuller (1993) shows a plot of G versus D (Figure 3) explain why minimization of Saber's equations 29 a to c are necessary to find an "equilibrium" state, rather than just minimization with respect to f_{ig} as shown by Weissmuller. Is this really an equilibrium state?

h) In Figure 5 of Saber, why does grain size increase with temperature, and why does it decrease with increasing α?