

Homework 10 Advanced Thermodynamics
Due Monday October 31, 2022

Grimvall G, Magyari-Köpe, Ozoliņš V Persson KA *Lattice instabilities in metallic elements* Rev. Mod. Phys. **84** 945-986 (2012) review dynamic stability of crystalline lattices based on the sign of the phonon frequency predicted by simulations such as DFT simulations. This approach leads to some interesting conclusions and predictions that are not available from consideration of Gibbs or Helmholtz free energy minimization though it must be said that the approach and review is opinionated. However, it should be clear that variable frequencies of vibrations can exist, but a negative frequency is not physically possible or even imaginable.

- a) Explain what dynamic instability is and how it differs from metastability. How can dynamic instability modify the results of a CALPHAD calculation (p. 974). How is dynamic instability involved in melting of a crystal?
- b) Grimvall states “*Often an instability is present only for small q , i.e., for long-wavelength phonons. We call it an elastic instability.*” How does the wavelength relate to the wavevector k or q ? What does a long-wavelength phonon have to do with elastic modulus? What does a short wavelength photon relate to? What is a Brillouin zone?
- c) What is a Hessian matrix in the context of phonons? (<https://www.tcm.phy.cam.ac.uk/castep/documentation/WebHelp/content/modules/castep/thcastepphonon.htm>) P. 948 in Grimvall.
- d) This paper discusses possible crystalline structures for transition metals and brings up the point that in one view they could all be FCC but, in many cases, BCC is the stable form. How can dynamic instabilities explain the observed crystalline lattices. How can dynamic instabilities explain differences in lattices for nanoparticles and for epitaxially grown crystals.
- e) Explain how equation (20) is obtained from equation (17). Do the calculations. (I think you need to remember that $d(\ln x) = dx/x$.)