Homework 10 Advanced Thermodynamics
Due October 30, 2023

Tohei T; Kuwabara A; Oba F; and Tanaka I *Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations* Phy. Rev. B **73** 064304 (2006) discuss the relationship between stiffness and heat capacity for various polymorphs.

  a) Explain the difference between hardness and stiffness. Which would relate to the heat capacity and why?
  b) What is the difference between optical and acoustic phonons? Which are related to stiffness and which to heat capacity?
  c) Tohei states that "*vibrational frequency is proportional to square root of the stiffness within the harmonic approximation*" Derive this relationship.
  d) Calculate the "Debye stiffness" for diamond and for graphite as mentioned by Tohei. What is the difference between this value and the actual stiffness?
  e) Tohei notes that Wunderlich "*reported that the heat capacity of graphite becomes smaller than diamond at above 1000 K*". Explain this observation.
  f) Derive Tohei's equation (3). How does it differ from the equation given in the text just before equation (2)?
  g) Explain how Tohei obtains the Debye temperature, θ_D.