

Homework 11 Advanced Thermodynamics
Due Tuesday November 10, 2020

Tohei T; Kuwabara A; Oba F; and Tanaka I *Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations* Phys. 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 the expression

$$W(h\nu/k_B T) = (h\nu/k_B T)^2 \exp(h\nu/k_B T) / [\exp(h\nu/k_B T) - 1]^2$$

Given just before Tohei’s equation (1).

- g) Explain how Tohei obtains the Debye temperature, θ_D .