

**Homework 12 Advanced Thermodynamics**  
**Due November 17, 2024**

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