
Exercise 1 *Debye temperature*

The Debye approximation is assuming a phonon dispersion with $\omega = vk$ where v is the sound velocity.

a) Calculate in two dimensions the density of state $D(\omega)$, the frequency cut-off ω_D and the Debye temperature T_D.

b) The sound velocity is given by $v = \sqrt{B/\rho}$ where B is the bulk modulus and ρ is the mass density. In a previous lecture we saw how argon is bonded together through van-der-Waals interaction and takes an fcc structure with nearest neighbour distance 3.76 Å. Assume $B \approx 75\epsilon/\sigma^3$ where (for Argon) $\epsilon \approx 10\,\mathrm{meV}$ and $\sigma = 4/1.09 \approx 4\,\text{Å}$ are the parameters of the Lennard-Jones potential. Show, using rough approximations, that $v \approx 1150\,\mathrm{m/s}$.

c) With this sound velocity, evaluate the Debye temperature for this material. (Remember that opposed to (a) we are now in 3D.)

Exercise 2 *Heat capacity - Debye approximation*

Let us again use the Debye approximation.

a) Calculate in one and two dimensions the temperature dependence of the heat capacity for the limit where T is much smaller than the Debye temperature.

b) The sound velocity of diamond is 12 000 m/s whereas lead has 2000 m/s. For a finite fixed temperature in the limit $T \ll T_\mathrm{D}$, which of the two materials will have the highest heat capacity? From our knowledge of the phonon dispersion of a mono-atomic 1D chain, give arguments as to why diamond has a higher sound velocity.

Exercise 3 *Heat capacity - Einstein model*

Einstein derived the expression

$$C = 3Nk_\mathrm{B}\left(\frac{\hbar\omega_0}{k_\mathrm{B}T}\right)^2 \frac{\exp\left(\frac{\hbar\omega_0}{k_\mathrm{B}T}\right)}{\left[\exp\left(\frac{\hbar\omega_0}{k_\mathrm{B}T}\right)-1\right]^2}. \tag{1}$$

a) In figure 1, the heat capacity of diamond is plotted as $\frac{C_p}{3Nk_\mathrm{B}}$ versus temperature. Einstein's model has just one free parameter: ω_0. Based on these data (given below), determine the energy scale $\hbar\omega_0$ that would give the best description of the experiment.

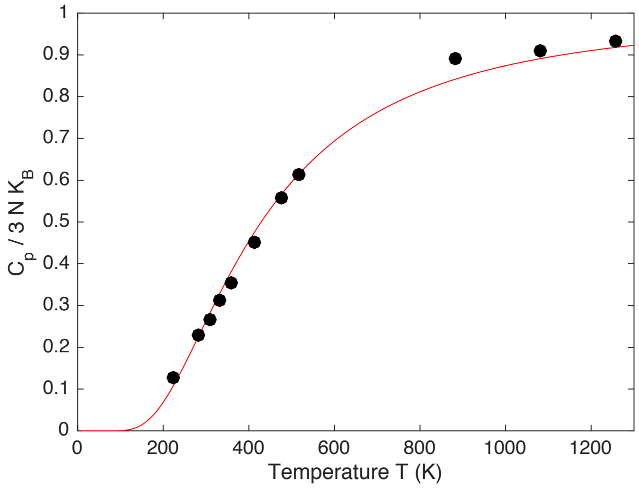

Figure 1: Heat capacity of diamond versus temperature T as of 1906. This was thus the information that Einstein had available when thinking about the problem of heat capacity.

b) How does this energy scale compare with the energy scale of optical phonons in diamond (see figure 2)?

The data points in figure 1 are:
T [K] = 222, 284, 308.5, 333, 358, 411, 477, 518, 880, 1080, 1259
$\frac{C_p}{3Nk_\mathrm{B}}$ = 0.1282, 0.2308, 0.2650, 0.3120 , 0.3547, 0.4530, 0.5556, 0.6154, 0.8932, 0.9103, 0.9316

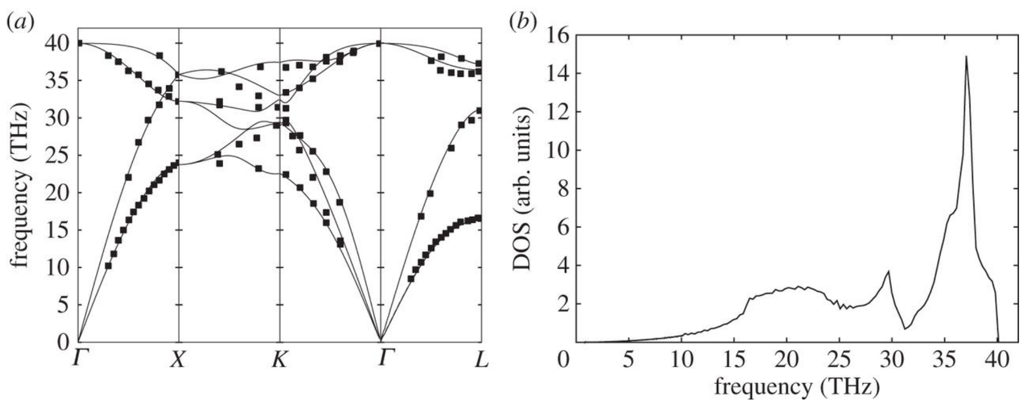

Figure 2: (a) Phonon spectrum of diamond. (b) Phonon density of states of diamond. From: http://rspa.royalsocietypublishing.org/content/470/2169/20140371