University of Zurich[UZH]

Solid State Physics
Exercise Sheet 6
Phonon thermal properties

HS19
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Received on 25th October
Discussed on 1st November

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 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 higher 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.

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

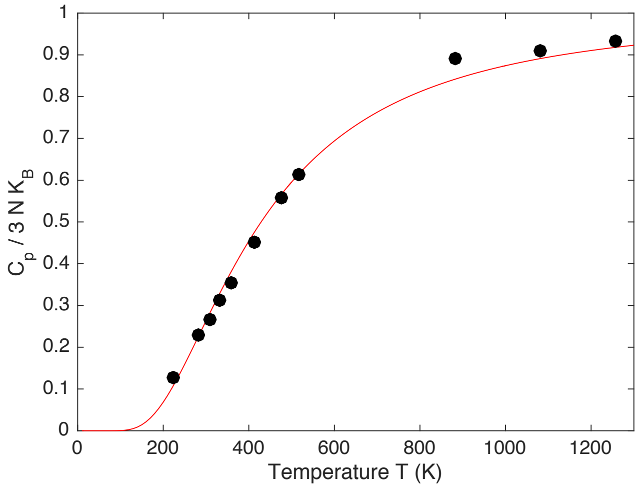

Figure 1: Heat capacity of diamond versus temperature T as of 1906. This was thus the information that Einstein had available when thinking about the problem of heat capacity.

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

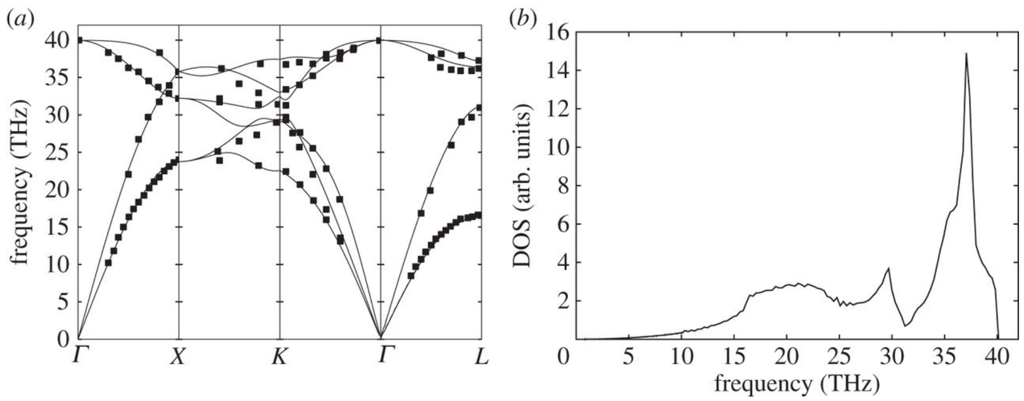

Figure 2: (a) Phonon spectrum of diamond. (b) Phonon density of states of diamond. From: http://rspa.royalsocietypublishing.org/content/470/2169/20140371