4). Acoustical phonons in a two-dim lattice

(a) Excluding zero point term, and assuming the two acoustic waves have the same velocity,

$$\langle U\rangle = 2\int_0^{\omega_D} <n_k> \hbar\omega_k D(\omega) = 2\int_0^{\omega_D} \frac{\hbar\omega_k D(\omega)\,d\omega}{e^{\hbar\omega/kT}-1}$$

2 polarizations, one longitudinal, one transverse

For each polarization $D(\omega) = \frac{dN(k)}{dk}\frac{dk}{d\omega}d\omega = \frac{d}{dk}\left[\left(\frac{L}{2\pi}\right)^2 \pi k^2\right]\frac{d\omega}{\upsilon} = \frac{A}{2\pi}\frac{\omega}{\upsilon^2}d\omega$

where we have $\omega = k\upsilon \rightarrow \textit{velocity of sound}$ and ω_D is defined by

$$N_C = \int_0^{\omega_D} D(\omega)d\omega = \int_0^{\omega_D}\frac{A\omega}{2\pi\upsilon^2}d\omega = \frac{A\omega_D^{\ 2}}{4\pi\upsilon^2}. \text{ Thus, } \langle U\rangle = \frac{A}{\pi\upsilon^2}\int_0^{\omega_D}\frac{\hbar\omega^2 d\omega}{e^{\hbar\omega/kT}-1}.$$

Define $x = \hbar\omega/kT \Rightarrow \langle U\rangle = \frac{A(kT)^3}{\pi\upsilon^2\hbar^2}\int_0^{x_D}\frac{x^2dx}{e^x-1}, x_D \equiv \frac{\hbar\omega_D}{kT}$.

(b) In the limit of low temperature, $x_D \equiv \hbar\omega_D/kT \rightarrow \infty$. And using the clue $\int_0^\infty \frac{x^2dx}{e^x-1} \approx 2.40$, we

find $\langle U\rangle \cong \frac{(2.40)A(k_BT)^3}{\pi\upsilon^2\hbar^2} = \frac{(2.40)(4N_C)(k_BT)^3}{\omega_D^{\ 2}\hbar^2} = \frac{9.6N_C(k_BT)^3}{\omega_D^{\ 2}\hbar^2}$

$$C_v \approx \frac{d\langle U\rangle}{dT} = \frac{7.20\cdot A\cdot k_B^{\ 3}T^2}{\pi\upsilon^2\hbar^2}$$

(c) In the limit high temperature $\frac{1}{e^x-1} \approx \frac{1}{x}$

So, $\langle U\rangle \approx \frac{A(k_BT)^3}{\pi\upsilon^2\hbar^2}\int_0^{x_D} xdx = \frac{A(k_BT)^3}{\pi\upsilon^2\hbar^2}\frac{x_D^{\ 2}}{2} = \frac{A(k_BT)\omega_D^{\ 2}}{2\pi\upsilon^2}$. But from definition of ω_D

in two dim in (a), we have $\omega_D^{\ 2} = \frac{4\pi N_C\upsilon^2}{A} \Rightarrow \langle U\rangle = 2N_Ck_BT$ and $C_v \approx \frac{d\langle U\rangle}{dT} = 2N_Ck_B$ (no surprise; this is just 2/3 of Dulong-Petit law in 3 dim).

5). Phonon propagation in quasi-two-dimensional crystal

(a) Phonon energy is found by assuming only phonons in the quasi-two-dim plane are important. Phonons propagating in vertical direction have a much larger ω vs. k so are not significantly populated. Furthermore, phonons propagating in the plane with transverse atomic motion directed normal to the plane are not significantly populated. Thus, each plane of solid contributes $\langle u\rangle_{plane} = \frac{A}{\pi\upsilon^2}\int_0^{\omega_D}\frac{\hbar\omega^2 d\omega}{e^{\hbar\omega/kT}-1}$.
In the limit of low temperature, this becomes

$$\langle u \rangle_{plane} = \frac{(2.40)A(k_B T)^3}{\pi \upsilon^2 \hbar^2}$$

and for the layered structure, $\langle u \rangle_{solid} = \langle u \rangle_{plane} \frac{t}{2.4\text{a}}$, $t \to$ sample thickness and $\frac{t}{2.4\text{a}}$ is the number of planes along vertical direction. So,

$$\langle u \rangle_{solid} = \frac{2.4At(k_B T)^3}{2.4\text{a}\pi \upsilon^2 \hbar^2} = \frac{V(k_B T)^3}{\text{a}\pi \upsilon^2 \hbar^2}.$$

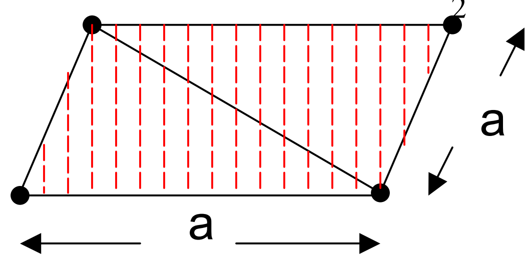
$V \to$ sample volume for a = 3 Ang, v = 5000 m/s, V = 1 cm^3 and T = 77 K. We get $\langle U \rangle_{solid} = 4.58 \times 10^{+6} \cdot V[J] = 4.58J$. And

$$C_v \approx \frac{d\langle u \rangle_{solid}}{dT} = \frac{3Vk_B{}^3 T^2}{\text{a}\pi \upsilon^2 \hbar^2} = 1.78 \times 10^5 \cdot V[J/k] = 0.178J/k$$

(a) at high temperatures $\langle U \rangle_{plane} = 2N_C k_B T$ where N_C is the number of primitive cells in the 2-D plane.

For a simple hexagonal lattice we know that the primitive cell area $A_{cell} = \frac{\sqrt{3}}{2}\text{a}^2$ where a is the lattice constant (see Kittel Chapter 2, Problem 2).

cell area $= 2 \cdot$ *area* of equilateral triangle, side a; *triangle area* $= \frac{\text{a}}{2} \cdot \text{a} \cos 60^0 = \frac{\sqrt{3}}{4}$



So, $N = \frac{A}{A_{cell}} = \frac{2A}{\sqrt{3}\text{a}^2}$ and $\langle U \rangle_{solid} = \frac{4A \cdot t \cdot k_B T}{\sqrt{3}\text{a}^2 (2.4\text{a})} = \frac{0.96 \cdot V_C k_B T}{\text{a}^3}$

So, $\langle U \rangle_{solid} = 0.49 \cdot T[J]$.

$$C_v \cong \frac{d\langle U \rangle}{dT} = \frac{0.96 \cdot V \cdot k_B}{\text{a}^3} = 0.49\left[J - k^{-1}\right]$$

6). A 3-dim lattice with four atoms per primitive cell

(a) The number of acoustical lattice waves is 3. The number of optical lattice waves is 9 . Of all the optical waves, 3 are longitudinal and 6 are transverse.

(b) From Eqn (14) of Notes 8, the total energy of acoustical phonons according to the Debye model is $\langle U_{tot} \rangle = \sum_{p=1}^{3} \frac{\hbar V}{2\pi^2 v_{s,p}^3} \left(\frac{k_B T}{\hbar}\right)^4 \int_0^{x_{D,p}} \frac{x^3 dx}{e^x - 1} = \sum_{p=1}^{3} 3N_C k_B T \left(\frac{k_B T}{\hbar \omega_D}\right)^3 \int_0^{x_{D,p}} \frac{x^3 dx}{e^x - 1}$ subject to the constraint $\omega_{D,p}{}^3 = \frac{6\pi^2 v_{s,p}{}^3 N_C}{V}$ where N_C is the number of unit cells, V is the volume of the crystal sample, and $v_{s,p}$ is the speed of sound for the pth wave type (i.e., polarization). In the limit of low temperature, $x_D = T_D/T$ gets very large so we can approximate $\int_0^{\infty} \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15}$. And we get $< U_{tot} >= \sum_{p=1}^{3} \frac{\pi^4}{5} N_C k_B T \left(\frac{k_B T}{\hbar\omega_D} \right)^3$. The heat capacity is $C_V \approx d<U_{tot}>/dT = = \sum_{p=1}^{3} \frac{4\pi^4}{5} N_C k_B \left(\frac{k_B T}{\hbar\omega_D} \right)^3$

(c) The Debye frequency is given by $\omega_{D,p}{}^3 = \frac{6\pi^2 v_{s,p}{}^3 N_C}{V}$ where N_C/V is the inverse volume of a primitive cell. Substitution of the sample parameters leads to $\omega_D = 6.3 \times 10^{13}\ s^{-1}$. Application of the relation $(k_B T_D / \hbar)^3 = \omega_{D,p}{}^3$ then yields $T_D = 479$ K.

(d) At 77 K we have $T < T_D$ so the low-temperature expression in (b) should be a good approximation, and the sum over polarizations p leads to a factor of 3 since all acoustic waves are assume to have the same speed of sound, 5000 m/s. This leads to the result $C_V{}' \equiv \frac{C_V}{V} \approx \frac{12\pi^4}{5} \frac{N_C}{V} \cdot k_B \left(\frac{T}{T_D} \right)^3 = 4.5 \times 10^5$ J/K.

(e) The classical (Dulong-Petit) heat capacity is given by $3N_c k_B$, and the specific heat capacity by $3(N_C/V)k_B = 1.38 \times 10^6$ J/K – 3 times larger than the 77-K value.