

Solutions for Homework 5

October 6, 2006

1 Energy to heat Al

The Dulong-Petit classical specific heat is $3Nk_B$ so that $\Delta U = 3Nk_B\Delta T = 6.023 \times 10^{23} \times 1.3806 \times 10^{-23} \times 3\Delta T = 8.315 \times 3\Delta T$. For $\Delta T = 10K$, $\Delta U = 250J$. For $\Delta T = 300K$, $\Delta U = 7484J$.

For the Debye theory, $U = 9Nk_B T (T/\Theta)^3 \int_0^{\Theta/T} dx \frac{x^3 e^x}{(e^x - 1)}$, where $\Theta_D = 428K$. Using Eq. 29, U is reduced from the classical value by the factor $3(T/\Theta)^3 \int_0^{428/300} dx \frac{x^3 e^x}{(e^x - 1)} = 3 \times 0.344 \times 0.546 = 0.564$ or $U = 4222J$. (Any value approximately correct will be accepted if the reasoning is correct.)

For low T we can use the form of the heat capacity given in Eq. 32 (derived using fact that the integral in Eq. 31 approaches the limit $\pi^4/15$) $C_V = 234Nk_B(T/\Theta)^3$, so that $U = (234/4)Nk_B T (T/\Theta)^3 = (234/12)(T/\Theta)^3 \times 3Nk_B T$, where the last expression is $(234/12)(T/\Theta)^3 \times U_{classical}$, with $U_{classical} = 3Nk_B T$ is the value calculated above. For $T = 10K$, the reduction factor is $(234/12)(T/\Theta)^3 = 19.5 \times 1.27 \times 10^{-5}$ and $U = 3.18 \times 10^{-3} J$.

Conclusion: Classical mechanics totally fails at low T where quantum effects are crucial. Quantum effects make changes of order a factor of 2 at room temperature.

2 Debye temperature and speed of sound

The formula for the Debye temperature in Kittel Eq 28 is $k_B\Theta = \hbar v(6\pi^2 N/V)^{1/3}$. For the diamond structure $N/V = 8/a^3$ so $(N/V)^{1/3} = 2/a$. Thus $v = \Theta \frac{k_B}{\hbar} \frac{a}{2} (\frac{1}{6\pi^2})^{1/3} = \Theta a \times 1.678 \times 10^{10} m/s$ with Θ in K and a in m. Thus we find:

Carbon: $a = 3.567 \times 10^{-10} m$, $\Theta = 2230K$, $v = 1.34 \times 10^4 m/s$

Silicon: $a = 5.43 \times 10^{-10} m$, $\Theta = 645K$, $v = 0.588 \times 10^4 m/s$

This compares to longitudinal speed in the (100) direction (see homework 4)

$$v = (C_{11}/\rho)^{1/2}.$$

For diamond, $C_{11} = 10.76 \times 10^{11} N/m^2$, $\rho = 3.52 \times 10^3 Kg/m^3$

$$v = (C_{11}/\rho)^{1/2} = 1.75 \times 10^4 m/s$$

For silicon, $C_{11} = 1.66 \times 10^{11} N/m^2$, $\rho = 2.33 \times 10^3 Kg/m^3$

$$v = (C_{11}/\rho)^{1/2} = 0.844 \times 10^4 m/s$$

Note that the longitudinal speed in the (100)direction is higher than the average v in the Debye expression. This is because the transverse speeds are lower so the average speed is lower than the longitudinal speed in the (100)direction.

3 What energy phonons contribute most to C_V at a given T ?

The phonons that contribute most to the heat capacity at temperature T (which is much below the Debye temperature) are ones with frequency at the maximum of the integrand in Eq. 30 of Chapter 5. This is because the contributions are additive and we only have to find the maximum. Consider the last form with the integrand $\frac{x^4 e^x}{(e^x - 1)^2}$. This is a function that increases as x^2 for small x (note the numerator $\propto x^4$ and the denominator $\propto x^2$). At large x , it decreases as $x^4 e^{-x}$. Therefore there is a maximum as long as T is low and the upper limit x_D is large. By plotting the function, I find the maximum to be roughly $x = 4$, i.e., $\hbar\omega = 4k_B T$.

4 Root mean square displacement

For Al $a = 0.286 \times 10^{-9} m$, so the nearest. neigh. distance is $R = a/2^{1/2} = 0.202 \times 10^{-9} m$. The mass is $M = 26.98 Amu = 0.451 \times 10^{-25} Kg$. Using the estimate $C = 100 eV/nm^2 = 16 J/m^2$, we find $CM = 7.17 \times 10^{-25} J^2 s^2/m^2$

(a) Find an estimate of the $T=0$ zero point motion

$$\Delta x_{rms} \approx (\hbar^2/CM)^{1/4} = (1.05^2 \times 10^{-68} / 7.17 \times 10^{-25})^{1/4} = 1.11 \times 10^{-11} m.$$

(b) For $T=1000K$ using the high temperature estimate $(2k_B T/C)^{1/2}$, we find $\Delta x_{rms} \approx 4.15 \times 10^{-11} m$.

(c) Both values are smaller the the nearest neighbor distance R , and the value at $1000K$ is about 20% of R , which is very reasonable since it is found empirically that solids melt when the value reaches 30%.

5 Kittel, Problem 5-1.

The density of states is the number of state per unit energy. using Eq. 15, $D(\omega) = \frac{L}{\pi} \frac{1}{d\omega/dk}$.

For the one dimensional chain, $\omega = (4C/M)^{1/2} \sin(ka/2)$ and the group velocity is $v_g = \frac{d\omega}{dk} = (a/2)(4C/M)^{1/2} \cos(ka/2)$. In terms of ω , $v_g = (a/2)(4C/M)^{1/2} (1 - \sin^2(ka/2))^{1/2}$. Thus

$$D(\omega) = \frac{L}{\pi} \frac{1}{d\omega/dk} = \frac{2N}{\pi} \frac{1}{(\omega_m^2 - \omega^2)^{1/2}}$$

where we used $\omega_m^2 = 4C/M$ and $\frac{2L}{\pi a} = \frac{2N}{\pi}$.

6 Thermal conductivity

Consider two crystals of identical size and shape but Debye temperatures differing by a factor of 2. Define the ratio $\Theta_2/\Theta_1 = 2$. Then $v_2/v_1 = 2$ and the heat capacity $C_{V2}/C_{V1} = 1/8$. Thus in the low temperature regime, where the thermal conductivity $K = CvL$ is limited by the surface scattering, the ratio of the thermal conductivities is $K_2/K_1 = 2/8 = 1/4$. Note that L is the same since it depends on the sample dimensions.