Problem set 9

Due May 7, 2025

1. Find in physicochemical tables the densities and sound velocities of copper and diamond and compute their Debye temperatures based on the formula derived during the lecture

$$\Theta_D = \frac{h v_\circ (6\pi^2 \rho)^{\frac{1}{3}}}{2\pi k_B} \tag{1}$$

   where $v_\circ$ is the sound velocity in the material and ρ is its atom-number density (expressed as the number of atoms per cubic meter), $h = 6.626 \times 10^{-34}$ J×s is the Planck constant, and $k_B = 1.3806 \times 10^{-23}$ J/(mol×K) is the Boltzmann constant.

   Find the Debye temperatures determined experimentally and compare with the calculated values. In each case state the source of the data.

2. Demonstrate that, in high-temperature limit, the expression for the oscillation contribution to the energy of the crystal in the Debye model

$$U = U_\circ + \frac{9 N k_B}{\Theta_D^3} T^4 \int_0^{\frac{\Theta_D}{T}} \frac{x^3}{e^x - 1} dx \tag{2}$$

   becomes that corresponding to the Dulong-Petit law.

3. (Additional problem for inquisitive students.) Based on the equation 2, derive the expression for the molar heat capacity expressed in the universal gas constant (R) units and make a plot of heat capacity in T/Θ_D. You will need to compute the integral numerically.