

HW#1 Problems – Thermodynamics and Statistical Mechanics

1. From a good table of materials properties, find the highest and lowest values of the following quantities for *elemental solids* at or near 300 K:

- (a) Compressibility in unit is Pa^{-1} .
- (b) Bulk expansivity (or CTE) in unit of T^{-1} .
- (c) Thermal conductivity at 300 K in unit of W/m-K .
- (d) Electrical conductivity in units of S/m .

2. One of the most important thermodynamic properties of solids is the linear expansivity (otherwise known as the coefficient of thermal expansion CTE), $\alpha \equiv (L)^{-1} (\partial L / \partial T)|_P$.

(a) Suppose a 1 cm^3 copper cube is used as a heat sink at 150°C and 1 Atm pressure. How much does the width (or height) of the cube increase relative to room temperature (300 K) in absolute units?

(b) Another important quantity is the isothermal hydrostatic compressibility $\kappa \equiv (V)^{-1} (\partial V / \partial P)|_T$. How much hydrostatic pressure would be required to achieve the same absolute reduction in width or height as the increase in (a) in units of MKSA and Atm?

(clues: for copper, the volumetric expansivity is $\beta = (V)^{-1} (\partial V / \partial T)|_P = 5 \times 10^{-5} / \text{K}$ and $\kappa = 8 \times 10^{-12} \text{ m}^2/\text{N}$; treat the copper as isotropic and homogeneous; $1 \text{ Atm} \approx 10^5 \text{ N/m}^2$; $0^\circ\text{C} = 273 \text{ K}$).

3. A 1 cm^3 of copper and 1 cm^3 of crystalline silicon are heated from 300 to 400 K.

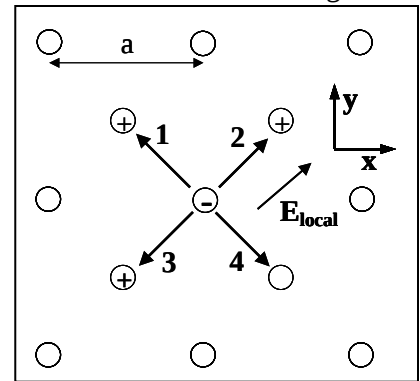
(a) What change of hydrostatic pressure would be required to keep the volume of each constant?

(b) Given the constant volume, what would the total heat input δQ for each cube be?

(c) What change of volume would be required to keep the hydrostatic pressure constant?

(Clues: assume bulk expansivities: copper $\beta = 55 \times 10^{-6} / \text{K}$; for Si $\beta = 8.4 \times 10^{-6} / \text{K}$; specific heat capacities: Cu = 387 J/kg-K , Si = 700 J/kg-K ; for Si $\kappa = 1.0 \times 10^{-6} \text{ atm}^{-1}$).

4. A two-dim solid at temperature T is in the form of a square lattice with nominal neutral atoms having an occasional defect. The defect consists of a negatively charged impurity ion that substitutes a normal atom (i.e. substitutional impurity) and a positively charged smaller impurity ion that goes into the lattice interstitially mid-way to the next-nearest neighbors of the square lattice. Assume that the positive ion is small enough to occupy any of the four interstitial sites with equal probability in the absence of external forces. Now apply a “local” electric field along the as shown to the right, and assuming that Maxwell-Boltzman statistics are valid.



- (a) Formulate the new probability of occupancy at each interstitial site.
- (b) Calculate the new occupancy probability for each state assuming $a = 3.0 \text{ \AA}$, $E = 1.0 \times 10^8 \text{ V/m}$ and $T = 300 \text{ K}$.

5. The venerable Maxwell-Boltzman pdf describes the probability of a particle having a velocity $\mathbf{v}$ when it is fully distinguishable from all other particles, has kinetic energy only, and this kinetic energy is given from Newton's law of motion as $u_K = m|\mathbf{v}|^2/2$: $P(\mathbf{v})d\mathbf{v} = (m/2\pi k_B T)^{3/2} \exp(-m\mathbf{v}^2/2k_B T)d\mathbf{v}$ where $v = |\mathbf{v}|$. [Note: this is very important in the development of the kinetic theory transport theory of charge carriers in metals and semiconductors, as will be covered in ECE215B].

(a) Derive the mean velocity $\langle \mathbf{v} \rangle$ using basic probability theory.

(b) Derive the “most likely” velocity $\mathbf{v}_{\text{max}}$ using calculus [i.e., where $P(\mathbf{v})d\mathbf{v}$ reaches its max].

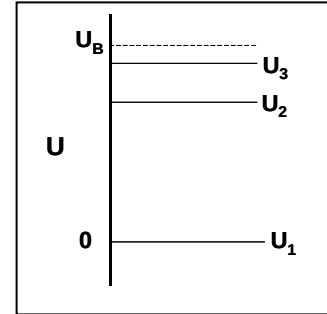
(c) Derive the variance of the velocity from the definition $(\Delta \mathbf{v})^2 = \langle (\mathbf{v} - \langle \mathbf{v} \rangle)^2 \rangle$, and from this calculate the rms deviation, $v_{\text{rms}} = [(\Delta \mathbf{v})^2]^{1/2}$.

(d) By integrating the $P(\mathbf{v})d\mathbf{v}$ over elevation and angle in spherical coordinates, find the function $M(v)dv$ – the Maxwellian *distribution* of velocity (not a pdf anymore because we have integrated partially over the independent variable space). Now plot $dM(v)/dv$ using your favorite graphical tool (e.g., Excel) for the fundamental particle of choice in electrical engineering – the electron – and use this plot to contrast the three characteristic velocities - the mean from (a), the most likely from (b), and the rms value from (c).

6. Suppose a spatially distinguishable particle of a solid is described by the three level energy structure shown to the right, and is in thermal equilibrium with the remainder of the solid at temp T . Suppose the energy levels are given by $U_n = U_B(1 - 1/n^2)$ (hydrogenic ladder).

(a) According to Boltzmann, which level has the highest probability of occupancy? Write an analytic expression for this probability in terms of U_B and $k_B T$. Evaluate numerically for $U_B = k_B T$.

(b) Which level has the lowest probability of occupancy? Write an analytic expression for this probability in terms of U_B and $k_B T$. Evaluate numerically for $U_B = k_B T$.



7. Heat capacity of two level system.

(a) Consider a two-level system with an energy splitting $k_B \Delta$ between upper and lower states. Derive an expression for the heat capacity. Is this a monotonic function or does it show a maximum?

(b) Plot the above heat capacity vs the parameter Δ/T using your favorite graphical tool. Then by graphical or numerical techniques, determine the value of Δ/T that produces the maximum C .