In-course Examination

Physics, CSE-1104

March 27,2019

Answer ALL questions Time: 1 hour 30 minutes [Marks 25]

1. Two moles of a monatomic ideal gas are caused to go through the cycle shown in the left figure below. Process bc is a reversible adiabatic expansion. Also $p_b = 10.4$ atm, $V_b = 1.22$ m^3 and $V_c = 9.13$ m^3. Calculate: (a) the heat added to the gas, (b) the heat leaving the gas, (c) the net work done by the gas, (d) the change of entropy in processes ca and ab, and (e) the efficiency of the cycle. [1+1+1+(1+1)+1=6]

   Solution: For monoatomic gas: $C_V = \frac{3}{2}R$, $C_P = C_V + R = \frac{5}{2}R$, $\gamma = C_P/C_V = 5/3 = 1.66$.

   (a) Energy added to the system during $a \to b$ is: $Q_{ab} = nC_V\Delta T = \frac{3}{2}nR\Delta T$.

   From $PV = nRT$ we get, $\Delta(PV) = P\Delta V + V\Delta P = nR\Delta T$

   Hence, $Q_{ab} = \frac{3}{2}V\Delta P = \frac{3}{2}V(P_b - P_a)$

   To get P_a, we use the equation of the adiabatic path: $P_bV_b^\gamma = P_cV_c^\gamma = P_aV_c^\gamma$.

   Hence, $P_a = P_b(\frac{V_b}{V_c})^\gamma = 10.4\text{atm} \times \left(\frac{1.22}{9.13}\right)^{1.66} = 0.36813 \quad \text{atm} = 0.36813 \times 1.01325 \times 10^5\text{Pa} = 3.7301 \times 10^4\text{Pa} = 0.36813\text{atm}$.

   Hence, $Q_{in} = Q_{ab} = \frac{3}{2}V_b(P_b - P_a) = \frac{3}{2} \times 1.22 \times (10.4 - 0.36813) \times 1.01325 \times 10^5 \quad \text{m}^3\text{Pa} = 1.524718 \times 10^6 \quad J$

   (b) $Q_{out} = Q_{ca} = nC_P\Delta T = \frac{5}{3}nR\Delta T = \frac{5}{3}P_a(V_a - V_c) = \frac{5}{3} \times 3.7301 \times 10^4\text{Pa} \times (1.22 - 9.13)\text{m}^3 = -4.91751 \times 10^5 J$

   Hence, $|Q_{out}| = 4.91751 \times 10^5 J$

   (c) For the cyclic process, $\Delta E_{int} = 0 \Rightarrow W = Q_{in} - |Q_{out}| = (1.524718 \times 10^6 - 4.91751 \times 10^5)J = 1.032967 \times 10^6 J$

   (d) (i) $\Delta_{ab}S = -\Delta_{ca}S$ since in the cyclic process $\Delta_{abca}S = 0$ and $\Delta_{bc}S = 0$.

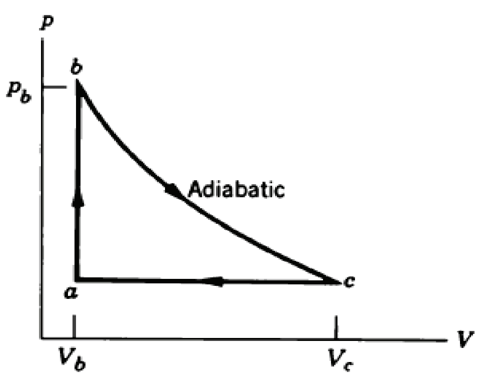
   Hence, for an ideal gas we get

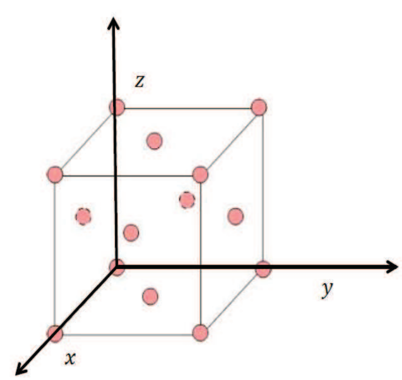
$$\Delta S = nR\ln\left(\frac{V_f}{V_i}\right) + nC_V\ln\left(\frac{T_f}{T_i}\right)$$

   which gives, for the process ab

$$\begin{aligned}\Delta_{ab}S &= nRln(1) + nC_V\ln\left(\frac{T_b}{T_a}\right) = nC_V\ln\left(\frac{nRT_b}{nRT_a}\right) = nC_V\ln\left(\frac{P_bV_b}{P_aV_a}\right)\\ \Delta_{ab}S &= nC_V\ln\left(\frac{P_b}{P_a}\right) = \frac{3}{2}R\ln\left(\frac{10.4}{0.36323}\right) = 41.83659 \quad J/K\end{aligned}$$

   (e) Efficiency $= W/Q_{in} = 1 - |Q_{out}|/Q_{in} = 100 \times \Big(1 - (4.91751 \times 10^5)/(1.524718 \times 10^6)\Big) = 67.74\%$





2. **Maxwell-Boltzmann Distribution:** The Maxwell-Boltzmann speed distribution formula is given by:

$$N_v(v) = 4\pi N\Big(\frac{m}{2\pi k_B T}\Big)^{3/2} v^2 e^{-mv^2/2k_BT}$$

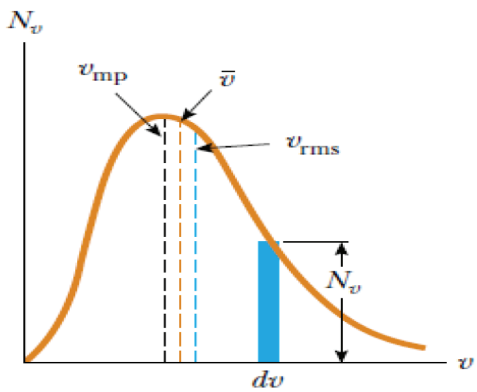
(a) Draw the above distribution with respect to speed of the molecules for different temperatures. Identify the most probable speed, average speed and the RMS speed in the figure. [1+1]

(b) From the speed distribution formula, derive the energy distribution formula assuming only kinetic energy as the internal energy of an ideal gas. [1]

(c) Hence derive the mean energy, the most probable energy and the RMS energy of an ideal gas in thermal equilibrium at temperature T. [1+1+1]
You may find the following integrals useful: $\int_0^\infty u^{3/2}e^{-u}\mathrm{d}u = (3/4)\sqrt{\pi}$, $\int_0^\infty u^{5/2}e^{-u}\mathrm{d}u = (15/8)\sqrt{\pi}$

(d) Is the most probable energy equal to $(1/2)mv_{mp}^2$, where m is the mass of a gas molecule and v_{mp} is the most probable speed? Explain. [1]

Solution: (a)



(b) We have, number of particles within speed v to $v+dv$ is equal to the number of particles within kinetic energy E to $E+dE$. Hence, using $E = \frac{1}{2}mv^2 \Rightarrow dE = mvdv \Rightarrow dv/dE = 1/(mv) = \frac{1}{m\sqrt{2E/m}} = \frac{1}{\sqrt{2mE}}$, we get

$$\begin{aligned}
n_E(E)dE &= N_v(v)dv \Rightarrow n_E(E) = N_v(v)dv/dE \\
n_E(E) &= 4\pi N\Big(\frac{m}{2\pi k_BT}\Big)^{3/2}(2E/m)e^{-E/k_BT}\frac{1}{\sqrt{2mE}} = 4\pi N\Big(\frac{1}{2\pi k_BT}\Big)^{3/2}\sqrt{2E}e^{-E/k_BT} \\
n_E(E) &= \frac{2N}{\sqrt{\pi}}\frac{1}{(k_BT)^{3/2}}E^{1/2}e^{-E/k_BT}
\end{aligned}$$

(c) From normalization, total number of particles:

$$\int_0^\infty n_E(E)dE = \frac{2N}{\sqrt{\pi}}\frac{1}{(k_BT)^{3/2}}\int_0^\infty E^{1/2}e^{-E/k_BT}dE = \frac{2N}{\sqrt{\pi}}\frac{1}{(k_BT)^{3/2}}(k_BT)^{3/2}\int_0^\infty x^{1/2}e^{-x}dx = \frac{2N}{\sqrt{\pi}}\frac{\sqrt{\pi}}{2} = N$$

where we have used:

$$\int_0^\infty x^{1/2}e^{-x}dx = \int_0^\infty te^{-t^2}2tdt = 2\int_0^\infty t^2e^{-t^2}dt = 2\sqrt{\pi}/4 = \sqrt{\pi}/2$$

(i) Mean energy

$$\begin{aligned}
\bar{E} &= \frac{\int_0^\infty En_E(E)dE}{\int_0^\infty n_E(E)dE} = \frac{2N}{\sqrt{\pi}}\frac{1}{(k_BT)^{3/2}}\frac{1}{N}\int_0^\infty EE^{1/2}e^{-E/k_BT}dE \\
\bar{E} &= \frac{2}{\sqrt{\pi}}\frac{1}{(k_BT)^{3/2}}\int_0^\infty x^{3/2}e^{-x}dx(k_BT)^{5/2} = \frac{2k_BT}{\sqrt{\pi}}\int_0^\infty t^3e^{-t^2}2tdt \\
\bar{E} &= \frac{4k_BT}{\sqrt{\pi}}\int_0^\infty t^4e^{-t^2}dt = \frac{4k_BT}{\sqrt{\pi}}\frac{3\sqrt{\pi}}{8} = \frac{3}{2}k_BT
\end{aligned}$$

(ii) Most probable energy E_p is found from

$$\begin{aligned}
\left.\frac{\partial n_E(E)}{\partial E}\right|_{E_p} &= 0 \Rightarrow \frac{2N}{\sqrt{\pi}}\frac{1}{(k_BT)^{3/2}}\left[(\frac{1}{2})E^{-1/2}e^{-E/k_BT} - \frac{E^{1/2}}{k_BT}e^{-E/k_BT}\right]_{E_p} = 0 \Rightarrow \frac{1}{2}E_p^{-1/2} - \frac{E_p^{1/2}}{k_BT} = 0 \\
\Rightarrow \frac{\frac{1}{2}k_BT - E_p}{E^{1/2}k_BT} &= 0 \Rightarrow E_p = \frac{1}{2}k_BT
\end{aligned}$$

(iii) The RMS energy is found from

$$\begin{aligned}
E^2_{RMS} &= \frac{\int_0^\infty E^2 n_E(E)dE}{\int_0^\infty n_E(E)dE} = \frac{2N}{\sqrt{\pi}}\frac{1}{(k_BT)^{3/2}}\frac{1}{N}\int_0^\infty E^2E^{1/2}e^{-E/k_BT}dE \\
E^2_{RMS} &= \frac{2}{\sqrt{\pi}}\frac{1}{(k_BT)^{3/2}}\int_0^\infty x^{5/2}e^{-x}dx(k_BT)^{7/2} = \frac{2(k_BT)^2}{\sqrt{\pi}}\int_0^\infty t^5e^{-t^2}2tdt \\
E^2_{RMS} &= \frac{4(k_BT)^2}{\sqrt{\pi}}\int_0^\infty t^6e^{-t^2}dt = \frac{4(k_BT)^2}{\sqrt{\pi}}\frac{15\sqrt{\pi}}{16} = \frac{15}{4}(k_BT)^2 \\
\Rightarrow E_{RMS} &= \sqrt{\frac{15}{4}}k_BT
\end{aligned}$$

(d) The most probable speed is $v_{mp} = \sqrt{2k_BT/m}$, while the most probable energy is $E_p = \frac{1}{2}k_BT$. Hence,

$$\frac{1}{2}mv^2_{mp} = \frac{1}{2}m\frac{2k_BT}{m} = k_BT \neq E_p$$

Hence, the most probable speed does not correspond to the most probable energy. This is because the density of states in energy E varies differently than the density of states with speed v.

3. **FCC Lattice:** Consider a cubic lattice with the edges of the conventional unit cell along the $x-$, $y-$ and $z-$axis and the length of an edge equal to a.

   (a) Draw the (100), (101) and (111) planes of the lattice within the unit cell. [0.5+0.5+0.5]

   (b) Draw all the members of the family of planes belonging to {100}. How many planes will be in this family? Write the Miller indices of all of them. [1.5]

   (c) How many members are in the families of planes {110} and {111}? [0.5+0.5]

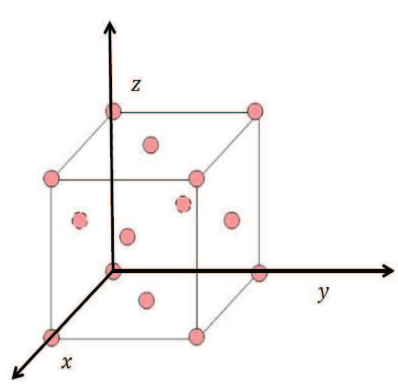
   (d) How many members are in the family of directions $< 100 >$, $< 110 >$ and $< 111 >$? Write the indices of all the members. [0.5+0.5+0.5]

   (e) The planar density of atoms is defined as the number of atoms per unit area in a particular plane. Considering the FCC lattice, find the planar density of atoms in the (100), (110) and (111) planes. [0.5+0.5+0.5]

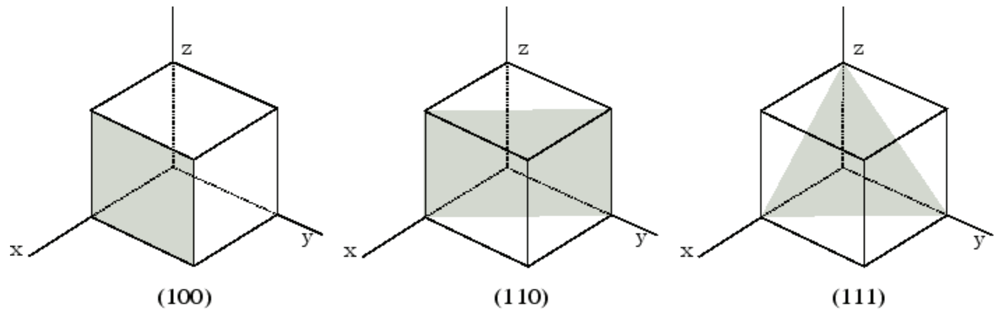
   (f) Considering the FCC lattice, calculate the packing fraction, if the atoms at the lattice points are considered as identical spheres. [2]

   (g) Find the reciprocal lattice vectors of the FCC lattice. [2]

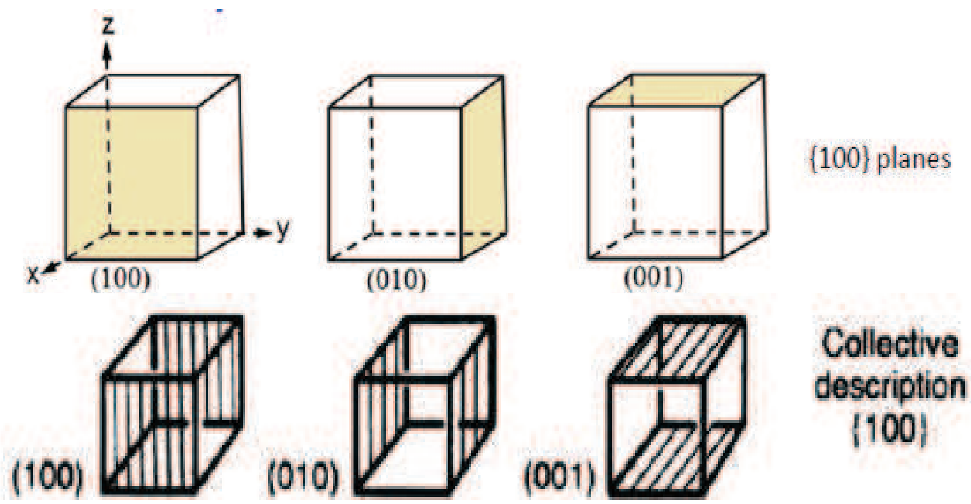
   (h) Identify in a clear figure the nearest neighbours of a particular atom in the FCC lattice. Find the distance to the nearest neighbours and the next-to-nearest neighbours. [0.5+(0.25+0.25)]



Solution: (a) The (100), (101) and (111) planes of the lattice within the unit cell:



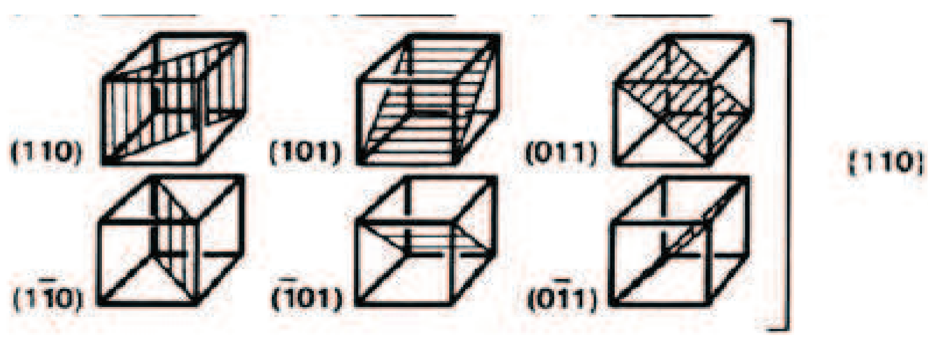
(b) The members of the family of planes belonging to {100}: There are six members: (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$

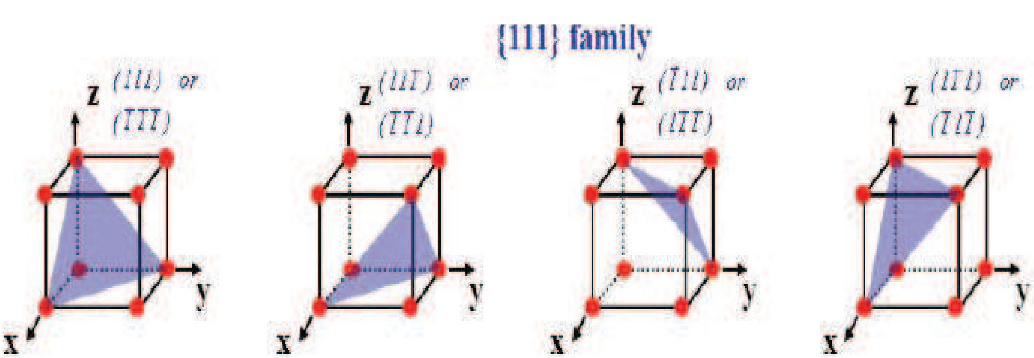


(c) The members in the families of planes {110} and {111} are:

$\{110\} = (110), (101), (011), (1\bar{1}0), (\bar{1}01), (0\bar{1}1)$

$\{111\} = (111), (\bar{1}11), (1\bar{1}1), (11\bar{1}), (\bar{1}\bar{1}1), (\bar{1}1\bar{1}), (1\bar{1}\bar{1}), (\bar{1}\bar{1}\bar{1})$





(d) The crystallographic directions are: $\langle 100\rangle = [100], [010], [001], [0\bar{1}0], [00\bar{1}], [\bar{1}00]$ six members.

$\langle 110\rangle = [110], [\bar{1}10], [1\bar{1}0], [\bar{1}\bar{1}0], [101], [\bar{1}01], [10\bar{1}], [\bar{1}0\bar{1}], [011], [0\bar{1}1], [01\bar{1}], [0\bar{1}\bar{1}]$ twelve members.

$\langle 110\rangle = [111], [\bar{1}11], [1\bar{1}1], [11\bar{1}], [\bar{1}\bar{1}1], [\bar{1}1\bar{1}], [1\bar{1}\bar{1}], [\bar{1}\bar{1}\bar{1}]$ eight members.

(e) The number of atoms in the planes are:

(i) (100) plane: There are four atoms on the corner of a (100) plane in fcc and one atom at the center. The radius of each atom is R whereas the length of the diagonal is $4R$.

Hence, $\sqrt{2}a = 4R \Rightarrow a = 2R\sqrt{2}$ Hence, planar density in (100) plane is:

$$PD_{100} = \frac{\text{No. of atoms}}{\text{Area of the plane}} = \frac{2}{8R^2} = \frac{1}{4R^2}$$

(ii) (110) plane: There are four atoms on the corner of a (110) plane in fcc and two atoms at the top and bottom edges. Again, the radius of each atom is R whereas the length of the diagonal is $4R$. Hence, $\sqrt{2}a = 4R \Rightarrow a = 2R\sqrt{2}$. Hence, planar density in (110) plane is:

$$PD_{110} = \frac{\text{No. of atoms}}{\text{Area of the plane}} = \frac{2}{8R^2\sqrt{2}} = \frac{1}{4R^2\sqrt{2}}$$

(iii) There are six atoms whose centers lie on this plane, which are labeled A through F. One-sixth of each of atoms A, D, and F are associated with this plane (yielding an equivalence of one-half atom), with one-half of each of atoms B, C, and E (or an equivalence of one and one-half atoms) for a total equivalence of two atoms. Now, the area of the triangle shown in the above figure is equal to one-half of the product of the base length and the height, h.

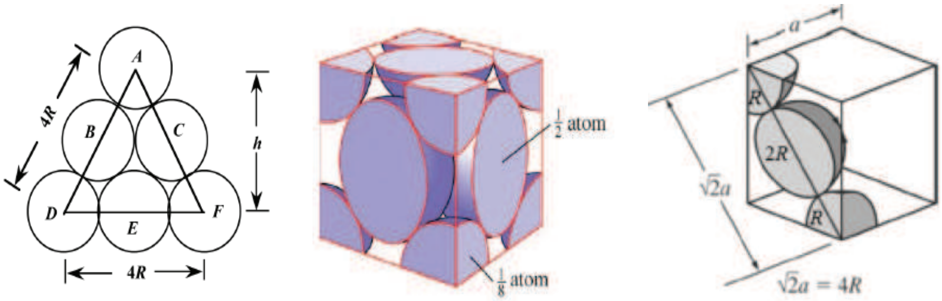
If we consider half of the triangle, then $(2R)^2 + h^2 = (4R)^2 \Rightarrow h = 2R\sqrt{3}$.

Area of the atoms in the plane:

$$A = \frac{1}{2}(4R)h = \frac{1}{2}(4R)(2R\sqrt{3}) = 4R^2\sqrt{3}$$

The planar density is:

$$PD_{111} = \frac{2}{4R^2\sqrt{3}} = \frac{1}{2R^2\sqrt{3}}$$



(f) Packing fraction: Number of atoms in a conventional cell is: $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 1 + 3 = 4$

Considering the atoms as hard spheres of radius R, total volume of the atoms is$= 4 \times \frac{4}{3}\pi R^3$

The relation between R and the fcc cell side a is $\sqrt{2}a = 4R$

Hence,

$$PF = \frac{16}{3}\pi R^3/a^3 = \frac{16}{3}\pi(\frac{\sqrt{2}}{4})^3 \approx 0.74$$

(g) For fcc lattice, the primitive unit vectors are:

$$\begin{aligned}
\vec{a} &= \frac{a}{2}(\hat{y} + \hat{z}) \\
\vec{b} &= \frac{a}{2}(\hat{x} + \hat{z}) \\
\vec{c} &= \frac{a}{2}(\hat{x} + \hat{y})
\end{aligned}$$

Volume of the primitive unit cell is:

$$V = |\vec{a}.\vec{b} \times \vec{c}| = \left(\frac{a}{2}\right)^3 |(\hat{y} + \hat{z}).(\hat{x} + \hat{z}) \times (\hat{x} + \hat{y})| = \frac{a^3}{8} |(\hat{y} + \hat{z}).(\hat{z} + \hat{y} - \hat{x})| = \frac{a^3}{4}$$

Hence,

$$\begin{aligned} \vec{a^*} &= \frac{\vec{b} \times \vec{c}}{\vec{a}.(\vec{b} \times \vec{c})} = \frac{a^2}{4}(\hat{x} + \hat{z}) \times (\hat{x} + \hat{y}) / \left(\frac{a^3}{4}\right) \\ \vec{a^*} &= \frac{1}{a}(\hat{z} + \hat{y} - \hat{x}) \end{aligned}$$

Similarly, we get,

$$\begin{aligned} \vec{b^*} &= \frac{1}{a}(\hat{z} - \hat{y} + \hat{x}) \\ \vec{c^*} &= \frac{1}{a}(-\hat{z} + \hat{x} + \hat{y}) \end{aligned}$$

(h) The nearest neighbour is a distance $2R$ away where the relation between R and the fcc cell side a is $\sqrt{2}a = 4R$. Hence the distance of the nearest neighbour is $a/\sqrt{2}$.

The distance of the next-to-nearest neighbour is a.