

# In-course Examination

## Physics, CSE-1104

March 08, 2018

1. Consider an ideal gas undergoing a reversible adiabatic compression or expansion.

(a) Starting from the first law of thermodynamics, show that

$$\text{i. } nC_V dT = nRT(dP/P) - nRdT \quad [2]$$

$$\text{ii. } nC_V dT = -nRT(dV/V) \quad [2]$$

Solution:

From the first law:  $dE_{int} = dQ_{in} + dW_{on} = dQ - PdV$

For adiabatic process  $dQ = 0$ .

[1/2]

For an ideal gas  $PV = nRT$  and  $nC_V = dE_{int}/dT$ .

Hence,  $PdV + VdP = nRdT$

[1/2]

Hence,

(i)  $dE_{int} = -PdV \Rightarrow nC_V dT = VdP - nRdT = PV(dP/P) - nRdT = nRT(dP/P) - nRdT$  [1] Hence, proved.

(ii)  $dE_{int} = -PdV \Rightarrow nC_V dT = -PV(dV/V) = -nRT(dV/V)$  Hence, proved. [2]

(b) Derive equations: (a) relating  $T$  and  $P$  using i. above and (b) relating  $T$  and  $V$  using ii. above, for the reversible adiabatic process (compression or expansion) of an ideal gas with constant heat capacities. Hence find the relation between (c)  $P$  and  $V$  for the adiabatic process. [1+1+1]

Solution:

(a) From i. above,  $nC_V dT = nRT(dP/P) - nRdT \Rightarrow n(C_V + R)(dT/T) = nR(dP/P)$  where  $C_V$  and  $C_P$  are molar heat capacities. Hence,

$$\begin{aligned} \frac{(C_V + R)}{R} dT/T &= dP/P \Rightarrow \frac{(C_V + R)}{R} \int dT/T = \int dP/P \Rightarrow \frac{C_P}{C_P - C_V} \ln T = \ln P \Rightarrow \frac{C_P/C_V}{C_P/C_V - 1} \ln T = \ln P \\ \frac{\gamma}{\gamma - 1} \ln T &= \ln P \Rightarrow \ln T = \frac{\gamma - 1}{\gamma} \ln P \Rightarrow \ln T = \ln P^{(\gamma-1)/\gamma} \\ T/P^{(\gamma-1)/\gamma} &= \text{constant} \Rightarrow \frac{T_1}{T_2} = \left( \frac{P_1}{P_2} \right)^{(\gamma-1)/\gamma} \end{aligned}$$

(b) From ii. above,  $nC_V dT = -nRT(dV/V) \Rightarrow C_V(dT/T) = -R(dV/V)$  where  $C_V$  and  $C_P$  are molar heat capacities. Hence,

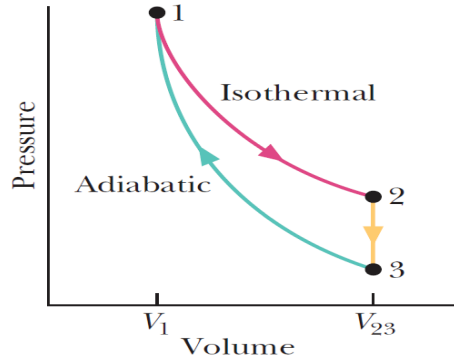
$$\begin{aligned} \frac{C_V}{(C_P - C_V)} \int dT/T &= - \int dV/V \Rightarrow \frac{1}{\gamma - 1} \ln T = - \ln V \Rightarrow \ln T = (1 - \gamma) \ln V \\ \ln T &= \ln V^{1-\gamma} \Rightarrow T/V^{1-\gamma} = \text{constant} \Rightarrow TV^{\gamma-1} = \text{constant} \\ \Rightarrow T_1 V_1^{\gamma-1} &= T_2 V_2^{\gamma-1} \end{aligned}$$

(c) From the above two results,

$$\begin{aligned} \frac{T_1}{T_2} &= \left( \frac{P_1}{P_2} \right)^{(\gamma-1)/\gamma} = \left( \frac{V_2}{V_1} \right)^{(\gamma-1)} \\ \left( P_1^{1/\gamma} V_1 \right)^{(\gamma-1)} &= \left( P_2^{1/\gamma} V_2 \right)^{(\gamma-1)} \Rightarrow P_1 V_1^\gamma = P_2 V_2^\gamma \Rightarrow PV^\gamma = \text{constant} \end{aligned}$$

2.  $n$  moles of a diatomic ideal gas are taken through the cycle with the molecules rotating but not oscillating, where  $V_{23} = 3.00V_1$ .

- (a) What are the values of  $p_2/p_1$ ,  $p_3/p_1$  and  $T_3/T_1$  ?  $[\frac{1}{2} \times 3 = 1.5]$   
 (b) For path  $1 \rightarrow 2$ , what are (i)  $W/nRT_1$ , (ii)  $Q/nRT_1$ , (iii)  $\Delta E_{int}/nRT_1$  and (iv)  $\Delta S/nR$ ?  $[\frac{1}{2} \times 4 = 2]$   
 (c) For path  $3 \rightarrow 1$ , what are (i)  $W/nRT_1$ , (ii)  $Q/nRT_1$ , (iii)  $\Delta E_{int}/nRT_1$  and (iv)  $\Delta S/nR$ ?  $[\frac{1}{2} \times 4 = 2]$   
 (d) Find the average speed, rms speed and the most probable speed of the gas at state 1 in terms of  $p_1$  and  $V_1$ .  $[\frac{1}{2} \times 3 = 1.5]$



Solution:

- (a) For the isothermal process,  $PV = nRT = \text{constant} \Rightarrow P_1V_1 = P_2V_{23} = P_23V_1 \Rightarrow P_2/P_1 = 1/3$ .

For the adiabatic process, with degrees of freedom  $f = 5$ ,  $C_V = f/2R = 5/2R$ ,  $C_P = 7/2R \Rightarrow \gamma_{dia} = 7/5 = 1.4$ , we get,  $PV^\gamma = \text{constant} \Rightarrow P_1V_1^\gamma = P_3V_{23}^\gamma = P_33^\gamma V_1^\gamma$ .

Hence,  $P_3/P_1 = 1/3^\gamma \approx 0.214798$

Again,  $T_1/T_3 = (P_1/P_3)^{(\gamma-1)/\gamma} \Rightarrow T_3/T_1 = (1/3^\gamma)^{(\gamma-1)/\gamma} = 1/3^{\gamma-1} \approx 0.644394$

- (b) For path  $1 \rightarrow 2$ ,  $W = \int_{V_1}^{V_{23}} (-PdV) = - \int_{V_1}^{V_{23}} nRT_1 dV/V = -nRT_1 \ln V_{23}/V_1 = -nRT_1 \ln 3$ .

Hence,  $W_{on}/nRT_1 = -\ln 3 \approx -1.01986$

Since, it is an isothermal process,  $\Delta E_{int} = 0$ . Hence from the first law, we get,  $Q_{in} = -W_{on} \Rightarrow Q/nRT_1 \approx 1.01986$

$\Delta E_{int}/nRT_1 = 0$ , during isothermal process for an ideal gas.

$\Delta S/nR = (Q/T_1)/nR = Q/nRT_1 \approx 1.01986$

- (c) During the isochoric process  $2 \rightarrow 3$ ,  $W_{2 \rightarrow 3} = 0$ .  $\Delta E_{int} = nC_V \Delta T = nC_V(T_3 - T_1) = nC_V T_1(T_3/T_1 - 1) = n(5/2)RT_1(1/3^{\gamma-1} - 1)$ .

During the cycle,  $\Delta E_{int} = 0$ . Hence, during  $3 \rightarrow 1$  we get  $\Delta E_{int-3 \rightarrow 1} = -\Delta E_{int2 \rightarrow 3}$  ( since  $\Delta E_{int1 \rightarrow 2} = 0$  ).

Thus,  $\Delta E_{int}/nRT_1 = (5/2)(1 - 1/3^{\gamma-1}) \approx 0.889$

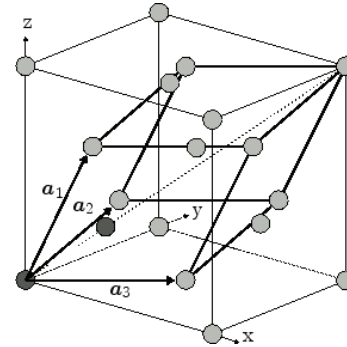
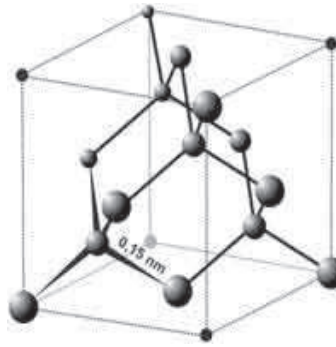
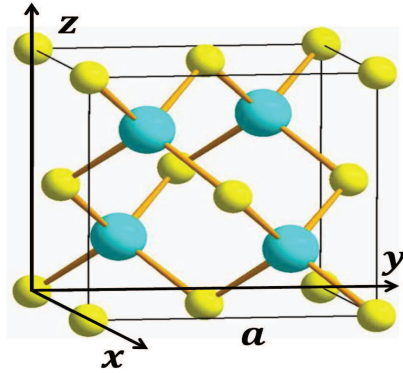
$Q/nRT_1 = 0$  during the adiabatic process, so also,  $S/nR$ .

$W/nRT_1 = \Delta E_{int}/nRT_1 \approx 0.889$  from the first law.

- (d) Average speed  $= \sqrt{8RT_1/(\pi M)} = \sqrt{8RP_1V_1/(\pi nM)}$ ,

RMS speed  $= \sqrt{3RT_1/(M)} = \sqrt{3RP_1V_1/(nM)}$

Most probable speed  $= \sqrt{2RT_1/(M)} = \sqrt{2RP_1V_1/(nM)}$



3. Consider the crystal structure of Sphalerite or Zinc Blend ( $\text{ZnS}$ ) as shown in the second figure above. The larger spheres represent S atoms and the smaller ones represent Zn atoms.

(a) Identify the type of the Bravais lattice. [1]

Solution: FCC lattice with a two-atom basis.

(b) Draw the three primitive lattice vectors  $\vec{a}_1, \vec{a}_2, \vec{a}_3$  and write them in terms of the Cartesian unit vectors  $\hat{x}, \hat{y}$  and  $\hat{z}$ . Taking the length of the side of the cube as  $a$ , find the volume of the primitive unit cell. [1 + 1 = 2]

Solution:  $\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$ ,  $\vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x})$ ,  $\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$

Volume of the primitive cell:  $V = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = (a^3/8)2 = a^3/4$

(c) Mark the basis of the crystal and find the position vectors of the atoms in the basis. [1 + 0.5 + 0.5 = 2]  
Solution: Position of atoms in the basis are: (0, 0, 0) for Zn atom and (1/4, 1/4, 1/4) for the S atom.

(d) Find the coordination number of the Zn and S atoms. [0.5 + 0.5 = 1]

Solution: For each of the atoms, the coordination number is 4. Each atom is at the center of a tetrahedron.

(e) If Zn and S atoms are replaced by carbon atoms, the above becomes the structure of diamond (c.f. third figure above). Assuming C atoms as hard spheres, find the packing fraction of the diamond structure. [3]  
Solution:

For the diamond structure, the basis atoms are the atoms at lattice points and a single atom displaced from the lattice point by a vector  $\vec{d} = (a/4)(\hat{x} + \hat{y} + \hat{z})$ .

Hence, the nearest neighbour distance  $d = (a/4)\sqrt{1^2 + 1^2 + 1^2}$ .

Four of the basis atoms sit inside the unit cube, 1/8 of the 8 corner spheres and 1/2 of the 6 face centered spheres (the same as FCC).

The packing fraction is therefore:

$$f = \frac{4 + (1/8) \times 8 + (1/2) \times 6}{a^3} V_{sph} = 8(4/3)\pi(d/2)^3/a^3 = 8\frac{4}{3}\pi\left(\frac{\sqrt{3}}{8}\right)^3 = \frac{\pi\sqrt{3}}{16}$$

(f) Find the Miller indices of a plane passing through three C atoms in the middle of the  $xy$ -,  $zx$ - and  $zy$ - planes (as shown in the figure). [2]

Solution: Consider a plane passing through a line joining the points  $(a, 0, 0)$ ,  $(0, 0, a)$  and the line passing through the points  $(a, 0, 0)$  and  $(0, a, 0)$ . This plane will contain also the line joining the points  $(0, a, 0)$  and  $(0, 0, a)$ .

Hence this plane will contain all three atoms in the middle of the  $xy$ -,  $zx$ - and  $zy$ - planes.

Hence the intercepts at the  $x$ -,  $y$ - and the  $z$ - axes are  $a, a, a$ .

Hence the Miller indices for this plane is (1, 1, 1).