UES-022 (Quantum Materials)
Department of Physics and Material Science, TIET
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Solutions Tutorial Sheet 4-5

1. $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$

2. At equilibrium,
   dW/dr = 0

   PE is between ions, so attractive interaction ≡ Coulomb interaction
   Hence, $A = 1/(4\pi\varepsilon_o) = 9 \times 10^9$

   Solving,

   $B = 3.905 \times 10^{-106}$ J-m^9

3. Bond length, $r_0 = r_a + r_c$ (r_c = radius of cation, r_a = radius of anion)
   Between ions the attractive interaction is coulomb interaction.
   So $$F = \frac{1}{4\pi\varepsilon_o}|z_1|.|z_2|\frac{e^2}{{r_0}^2}$$
   Solving,
   $r_0 = 0.2486$ nm $r_c = 0.0646$ nm

4. % covalent character = (C-M no./4.0) x 100

   Solving
   % metallic character for W = 3.5 %

5. $$\%\ ionic\ character = \left[1 - e^{-\frac{1}{4}(X_B - X_B)^2}\right] x\ 100$$ (Pauling's Equation)
   X_A: electronegativity of Atom A

   TiO_2: 51.4 %
   ZnTe: 6%

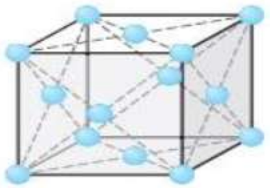
6. PPTs

7. PPTs

8. PPTs

9. $$Atomic\ packing\ fraction, APF = \frac{Volume\ occupied\ by\ atoms}{Volume\ of\ the\ unit\ cell}$$

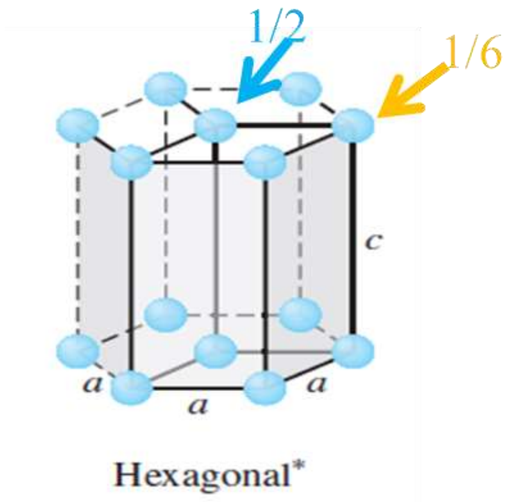
   $$Volume\ occupied\ by\ atoms = N\ x\ \frac{4}{3}\pi r^3$$

a) FCC  $\sqrt{2}a = 4R$

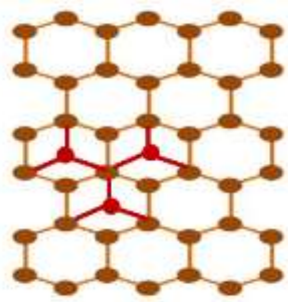
$$N = \frac{1}{8} x\, 8 + \frac{1}{2} x\, 6$$

APF = 0.74

b) Simple Hexagonal unit cell with c = 1.63 a
Let us consider the larger hexagonal unit cell consisting of 3 bravis lattice unit cells:



N = 2 x (1/2) + 12 x (1/6) = 3



Top view

For hex unit cell, 2r = a, and c = 1.63a = 1.63 x 2 r

APF = 0.37
Note: APF will change if the value of c changes.

10. $$Density = \frac{N\ x\ At\ mass\ /N_A}{Volume\ of\ the\ unit\ cell}$$

For FCC, N = 4
Vol of unit cell = a^3

Solving, a =0.359 nm
Also √2 a = 4 r
R = 0.128 nm

11. $v_d = \mu E$

Solving, E = 3.75 x 10^3 V/m

12. z = valency (for transition metals, it is taken to be the smaller one, eg for Fe: z = 2)

$$N_d = \frac{Density\ x\ N_A}{At\ mass}$$

Solving, $N_d = 8.39 \times 10^{28}$ /m^3

$n = z \cdot N_d = 16.77 \times 10^{28}$ electrons/m^3

13. PPTs

14. $\mu = \frac{e\tau}{m}$ = 0.756 x 10^{-2} m^2/Vs

$\sigma = \frac{ne^2\tau}{m} = ne\mu = 15.97\ x\ 10^6\ S/m$

Where

$n = z \cdot N_d = 1.32 \times 10^{28}$/m^3

15. PPTs

16. Only electrons near Fermi energy (E_f) contribute to conduction.

So

Energy, $E = E_f$

Velocity = v_f = 1.44 x 10^6 m/s, where $E_f = mv_f^2/2$

Momentum = pf = m• v_f = 13.1 x 10^{-25} kg m/s

17. $E_f = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$ = 2.1 eV

18.

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2} E^{1/2}$$

19.

$$E_f = k_B T$$

$T_f = 3.722 \times 10^4$ K

20.

$$Fraction\ of\ electrons\ effected = \frac{Energy\ Supplied}{Total\ Energy} = \frac{k_B T}{E_f}$$