Name ______________________________ Fall Semester, 2002

UNIVERSITY OF CALIFORNIA
College of Engineering
Department of Materials Science and Engineering

# Engineering 45

## Exam #1 (75 pts.)

1) Short answer.

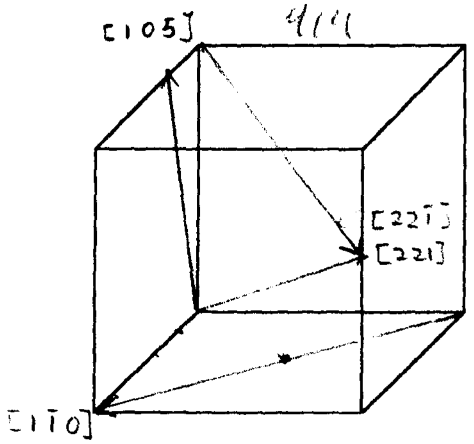
a) (6 pts.) Name the three primary bond types. Indicate if each bond type involves electron sharing or electron transfer and if the bond is directional or non-directional.

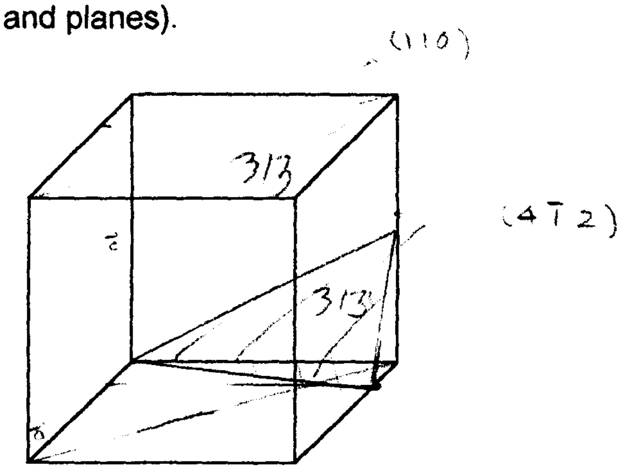
covalent bond : shared e⁻'s directional
ionic bond : electron transfer , non-directional
metallic bond electrons moving . non-directional

6/6

b) (10 pts) Using the two cubes provided, sketch the directions and planes listed below each. Be sure to clearly label your sketches (directions and planes).

10/10




[1 1̄ 0], [221], [22 1̄], [105]

(110), (4 1̄ 2)

c) (4 pts.) Give a direction within the family of <411> directions that is orthogonal to both [1 1̄ 0] and [22 1̄].

2/4

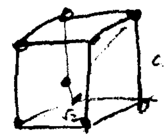
$$\cos\delta = \frac{uu' + ww' + vv'}{\sqrt{u^2+v^2+w^2}\,\sqrt{u'^2+w'^2+v'^2}}$$

The desired member of <411> with
has cos δ = 0 w/ both [1 1̄ 0] & [2 2 1̄]

[114] or [1̄ 1̄ 4]

d) (6 pts.) Chromium (Cr) and nickel (Ni) have the same atomic radius of 1.25 Å but differ in structure, Ni being fcc and Cr being bcc. Calculate the atomic density for Cr and Ni. Your answer should be in units of atoms/$cm^3$.

Cr: bcc



$1 Å = 10^{-10} m = 10^{-8} cm$

$1 Å = 10^{-10} m$

body diagonal $= \sqrt{3}a = 4r_{Cr}$

$\Rightarrow a = \frac{4}{\sqrt{3}} r_{Cr}$

$\rho = \frac{2 \text{ Cr atom}}{a^3} = \frac{(2) \text{ Cr atom}}{\left(\frac{4}{\sqrt{3}} \times 1.25 \times 10^{-10} m \times \frac{10^2 cm}{1m}\right)^3} =$ ~~$8.31 \times 10^{23}$ atom/$cm^3$~~

(3)

Ni: fcc, $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$ atom/unit cell

$\sqrt{2}a = 4r_{Ni} \Rightarrow a = \frac{4r_{Ni}}{\sqrt{2}}$

$\rho = \frac{4 \text{ atom}}{a^3} = \frac{(4) \text{ atom}}{\left[\frac{4}{\sqrt{2}}(1.25 \times 10^{-8} cm)\right]^3} =$ ~~$7.24 \times 10^{23}$ atom~~/$cm^3$

$9.05 \times 10^{22}$ atom/$cm^3$

e) (6 pts.) Beryllium (Be) has a hexagonal close packed (hcp) structure with a **c/a** ratio of 1.58. Calculate the atomic packing factor (APF) for Be. Assume that the lattice parameter **a** is equal to twice the atomic radius of Be, $r_{Be}$.

hcp has 2 atoms per unit cell.

0

2) BaO has the NaCl crystal structure with a lattice parameter of 5.50 Å. $O^{2-}$ has an ionic radius of 1.32 Å.

a) (2 pts.) What is the Bravais lattice associated with BaO? 2

fcc, with 2 atom per lattice point

b) (4 pts.) What is the ionic radius of $Ba^{2+}$?

$a = 5.50 Å = 2r_{O^{2-}} + 2r_{Ba^{2+}}$

$r_{Ba^{2+}} = \frac{a - 2r_{O^{2-}}}{2}$

$= \frac{5.50 Å - 2(1.32 Å)}{2}$

$= 1.43 Å$

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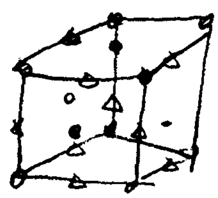
c) (5 pts.) What is the ionic packing factor (IPF) of BaO?

$IPF = \frac{4 \times \frac{4}{3}\pi (r_{Ba^{2+}}^3 + r_{O^{2-}}^3)}{a^3}$

$= \frac{\frac{16}{3}\pi [(1.43)^3 + (1.32)^3]}{(5.50)^3}$

$= 0.52\underline{6}1$

$\approx \boxed{0.526}$



NaCl type.

4 $Na^+$

4 $Cl^-$

$Na^+ = \frac{1}{8} \times 8 + 6 \times \frac{1}{2} = 4$

$Cl^- = \frac{1}{4} \times 12 + 1 = 4$

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3) You have discovered an unknown crystalline substance whose external morphology indicates that it is a cubic material. A diffraction pattern of this material, using radiation of wavelength 1.54 Å, provides the following data for the first six reflections:

| diffraction peak number | diffraction angle, θ |
|---|---|
| 1 | 13.70° |
| 2 | 15.97° |
| 3 | 22.85° |
| 4 | 27.05° |
| 5 | 28.30° |
| 6 | 33.15° |

a) (8 pts.) Is this material simple cubic (sc), body-centered cubic (bcc), or face-centered cubic (fcc)? Recall that diffraction occurs for all planar indices *h, k, and l* for sc, for *h+k+l*=even number for bcc, and for unmixed *h, k,* and *l* (i.e., either all odd or all even) for fcc. For cubic materials $d_{hkl}=a/(h^2+k^2+l^2)^{1/2}$.

bcc: h + k + l = even → smallest θ corresponds to (110) (200)

fcc: h, k, l unmix. → (111), (200)

$n\lambda = 2d\sin\theta$

$$\frac{d_1}{d_2} = \frac{\frac{\lambda}{2\sin\theta_1}}{\frac{\lambda}{2\sin\theta_2}} = \frac{\sin\theta_2}{\sin\theta_1} = \frac{\frac{a}{\sqrt{h_1^2+k_1^2+l_1^2}}}{\frac{a}{\sqrt{h_2^2+k_2^2+l_2^2}}} = \frac{\sqrt{h_2^2+k_2^2+l_2^2}}{\sqrt{h_1^2+k_1^2+l_1^2}} = 1.16$$

bcc: $\frac{\sqrt{h_2^2+k_2^2+l_2^2}}{\sqrt{h_1^2+k_1^2+l_1^2}} = \frac{\sqrt{4+0+0}}{\sqrt{1+1+0}} = \frac{2}{\sqrt{2}} = 1.41$

fcc: $\frac{\sqrt{4+0+0}}{\sqrt{1+1+1}} = 1.154$ ~ close to 1.16

So. it's fcc.

b) (4 pts.) What is its lattice parameter?

$a = \frac{4r}{\sqrt{3}}$ ← atom radius   $d_{111} = \frac{\lambda}{2\sin\theta_{111}}$

For fcc,

$$a = d_{111}\sqrt{1+1+1} = \frac{\lambda}{2\sin\theta_{111}}\sqrt{3}$$

$$= \frac{1.54 \text{ Å}}{2\sin 13.7°} \times \sqrt{3} = 5.63 \text{ Å}$$

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4) Ge and GaAs are semiconductors with energy band gaps of 0.66 eV and 1.4 eV, respectively. At 300 K the intrinsic resistivity $\rho_i$ of Ge and GaAs is 50 ohm-cm and $3 \times 10^8$ ohm-cm, respectively. Copper (Cu) is a metal with a resistivity of $8 \times 10^{-6}$ ohm-cm at 300 K in its pure form.

a) (5 pts.) Explain why the resistivities of Ge, GaAs, and Cu differ so much at this temperature. At same temp

Ge: intrinsic semiconductor $E_g = 0.66 eV$

GeAs: extrinsic semiconductor, $E_g = 1.4 eV$ largest $E_g$. R ← largest

Cu: conductor, VB and CB overlap. $E_g$ very small ← R smallest

Eactivation of e's is very small;

b) (5pts.) What is the resistivity of pure copper at 1000 K? Assume that its resistivity approaches zero at 0 K.

T= 300k $\rho_{rt} = 8 \times 10^{-6}\ \Omega\text{-cm}$

$$\rho = \rho_{rt}[1 + \alpha(T - T_{rt})]$$

at T = 0K

$$\rho = 0 = \rho_{rt} + \rho_{rt} \cdot \alpha(-T_{rt}) \qquad 1 + \alpha(-T_{rt}) = 0$$

$$\Rightarrow \alpha = \frac{1}{T_{rt}} = \frac{1}{300\ k}$$

$$\rho_{1000k} = 8 \times 10^{-6}\ \Omega \cdot cm \left[1 + \frac{1}{300k}(1000k - 300k)\right]$$

$$= 2.667 \times 10^{-5}\ \Omega \cdot cm$$

$$\approx \boxed{2.7 \times 10^{-5}\ \Omega \cdot cm}$$

c) (5 pts.) What is the resistivity of Ge at 1000 K. Recall that the intrinsic carrier concentration in a semiconductor $n_i$ is given by $n_i=n_0\exp[-E_G/(2kT)]$, where $n_0$ is a constant, $E_G$ is the energy band gap and $k$ is equal to $8.62\times10^{-5}$ eV/K.

$\rho = 50\ \Omega\cdot cm$

$\sigma = \frac{1}{50}\ \Omega^{-1}cm^{-1}$

$\sigma =$

$\sigma = \sigma_0 e^{-\frac{E_g}{2kT}}$

$\sigma_0 = \sigma e^{E_g/2kT}$

$= \frac{1}{50} \cdot e^{\frac{(0.66eV)}{2(8.62\times10^{-5} eV/K)(300K)}}$

$\sigma' = \sigma_0 e^{-\frac{E_g}{2kT'}}$

$= \sigma e^{E_g/2kT} \cdot e^{-E_g/2kT'}$

$= \sigma e^{\frac{E_g}{2k}(\frac{1}{T} - \frac{1}{T'})}$

$= \frac{1}{50} e^{\frac{0.66eV}{2(8.62\times10^{-5})}} \rightarrow (\frac{1}{300K} - \frac{1}{1000K})\ \Omega^{-1}cm^{-1}$

$= 151\ \Omega^{-1}cm^{-1}$

$\rho' = \frac{1}{\sigma'} = 0.0066\ \Omega\cdot cm$

5/5

d) (5 pts.) In an intrinsic semiconductor the Fermi energy, $E_F$, is located in the middle of the energy band gap, $E_G$. However, the introduction of donor impurities moves the Fermi energy toward the conduction band and at a particular temperature $E_F$ coincides with the donor energy level $E_D$. If the sulfur donor concentration $N_D$ in a GaAs crystal is $2\times10^{13}\ cm^{-3}$, at what temperature will $E_F$ coincide with $E_D$? In the extrinsic region the carrier concentration n is given by $n=N_D\exp[-(E_G-E_D)/kT]$, where $E_G-E_D$ is equal to 0.007 eV for sulfur donors.

$n_e = N_D$

If $E_F = E_D$, ~~conducting~~ charge carrier which contribute to conduction is $\frac{1}{2}$ of the ~~total~~ charge carrier ~~at $E_1$~~

$\because f(E) = \frac{1}{e^{(E-E_F)/kT}+1} = \frac{1}{2}$

Total charge carrier = $N_D$

~~extrinsic: $\sigma = \mu_e q_e n_e$~~

~~intrinsic: $= \sigma_0 e^{-(E_g-E_D)/2kT}$~~ $= \sigma = \mu_e q_e n_e$

Find T

$n = N_D e^{-(E_g-E_D)/kT} = N_D$

$e^{-(E_g-E_D)/2k} = 1 \Rightarrow -\frac{E_g-E_D}{2k} = 0 - E_F = E_D$

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