Solutions

**Fall Semester, 2002**

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

## Engineering 45

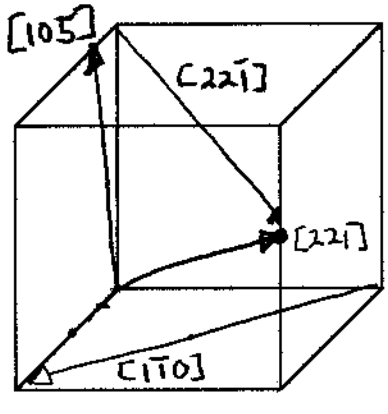
## Exam #1 (75 pts.)

1) Short answer.

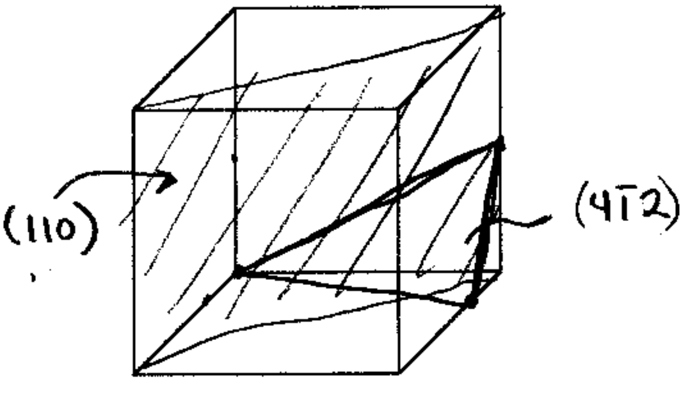
a) (6 pts.) Name the three primary bond types. Indicate if each bond type involves electron sharing or electron transfer and if the bond is directional or non-directional.

Ionic – electron transfer, non-directional
Covalent- electron sharing, directional
Metallic- electron sharing non-directional

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).



$[1\bar{1}0]$, $[221]$, $[22\bar{1}]$, $[105]$



$(110)$, $(4\bar{1}2)$

$\frac{1}{4}\ \bar{1}\ \frac{1}{2}$

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

$[114]$ The Direct product of these and $[1\bar{1}0]$ and $[22\bar{1}]$ is zero.

$[\bar{1}\bar{1}\bar{4}]$

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$^3$.

For bcc, the lattice constant $a = \frac{4r}{\sqrt{3}}$

$$\therefore \rho_{Cr} = \frac{2 \text{ atoms/unit cell}}{a^3 \text{ cm}^3\text{/unit cell}} = \frac{2}{\left(\frac{4}{\sqrt{3}} \times 1.25\times10^{-8}\right)^3} = 8.31\times10^{22} \frac{\text{atoms}}{\text{cm}^3}$$

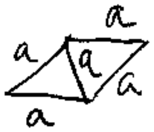
For fcc, the lattice constant $a = \frac{4r}{\sqrt{2}}$

$$\therefore \rho_{Ni} = \frac{4 \text{ atoms/unit cell}}{a^3 \text{ cm}^3\text{/unit cell}} = \frac{4}{\left(\frac{4}{\sqrt{2}} \times 1.25\times10^{-8}\right)^3} = 9.05\times10^{22} \frac{\text{atoms}}{\text{cm}^3}$$

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 sell.

$$\therefore APF = \frac{2\left(\frac{4}{3}\pi r^3\right)}{\text{Volume of cell}}$$



Volume of cell = Area of base × C

Area of base $= 2\left(\frac{1}{2}a * \frac{\sqrt{3}}{2}a\right) = \frac{\sqrt{3}}{2}a^2$ where $a = 2r$

$$\therefore APF = \frac{8\pi r^3}{3\times C\times 2\sqrt{3}r^2} = \frac{\overset{2}{\cancel{8}}\pi \cancel{r^3}}{\underset{3}{\cancel{6}}\sqrt{3}\cancel{r^2}(1.58\times\cancel{2r})} = \frac{2\pi}{3\sqrt{3}\times1.58}$$

$APF = 0.765$

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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?

FCC

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

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

$$r_{Ba^{2+}} = \frac{5.50 - 2(1.32)}{2} = 1.43\text{Å}$$

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

$$IPF = \frac{4\left[\frac{4}{3}\pi r_{Ba^{2+}}^3 + \frac{4}{3}\pi r_{O^{2-}}^3\right]}{a^3}$$

$$= \frac{16}{3}\frac{\pi}{a^3}\left(r_{Ba^{2+}}^3 + r_{O^{2-}}^3\right)$$

$$= \frac{16}{3}\frac{\pi}{5.5^3}\left(1.43^3 + 1.32^3\right) = 0.53$$

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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 | $\sin^2\theta$ |
|---|---|---|
| 1 | 13.70° | 0.0561 |
| 2 | 15.97° | 0.0757 |
| 3 | 22.85° | 0.1508 |
| 4 | 27.05° | 0.2068 |
| 5 | 28.30° | 0.2248 |
| 6 | 33.15° | 0.2990 |

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 $d_{hkl}=a/(h^2+k^2+l^2)^{1/2}$.

$$\lambda = 2d\sin\theta \therefore \lambda^2 = \frac{4a^2}{h^2+k^2+l^2}\sin^2\theta$$

$$\Rightarrow (h^2+k^2+l^2)\frac{\lambda^2}{4a^2} = \sin^2\theta$$

$$\boxed{\text{fcc}}$$

| Exp $\frac{\sin^2\theta}{\sin^2\theta_1}$ | $h^2+k^2+l^2$ sc | bcc | fcc |
|---|---|---|---|
| $\frac{1}{1} = \frac{3}{3}$ | (100) $1/1$ | (110) $2/2$ | (111) $3/3$ |
| $\frac{1.35}{1} = \frac{4.05}{3}$ | (110) $2/1$ | (200) $4/2$ | (200) $4/3$ |
| $\frac{2.69}{1} = \frac{8.06}{3}$ | (111) $3/1$ | (211) $6/2$ | (220) $8/3$ |

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

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

$$\therefore d = \frac{\lambda}{2\sin\theta} \text{ for } \theta_1 = 13.70°$$

$$d = 3.25\text{Å} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{a}{\sqrt{3}}$$

$$\therefore a = 5.63\text{Å}$$

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 $3\times10^8$ ohm-cm, respectively. Copper (Cu) is a metal with a resistivity of $8\times10^{-6}$ ohm-cm at 300 K in its pure form.

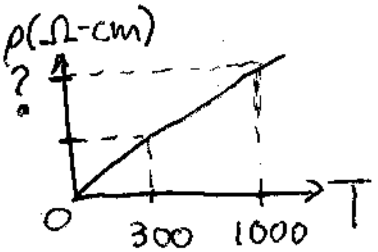
a) (5 pts.) Explain why the resistivities of Ge, GaAs, and Cu differ so much at this temperature.

The resistivity of Cu is significantly smaller than those of Ge and GaAs because Cu is a metal, possessing a high, temperature-independent electron concentration. On the other hand Ge and GaAs are semiconductors for which the intrinsic carrier concentration depends exponentially on the band gap energy ($n_i \propto e^{-E_g/2kT}$). Therefore, Ge, the material with a smaller bandgap, has a higher carrier density (actually some 7 orders of magnitude higher!) and a lower resistivity since resistivity $\rho = \frac{1}{q\mu n}$

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

For a metal the resistivity depends linearly on T.

At $T = 0K, \rho \to 0 \therefore$



$$\rho = mT + b, \; b = 0$$

$$m = \frac{\rho(T=300)}{T(T=300K)} = \frac{8\times10^{-6}}{300} = 2.67\times10^{-8} \; \frac{\Omega\text{-cm}}{K}$$

$$\rho = 2.7\times10^{-5} T$$

$$\therefore \rho_{1000} = 2.7\times10^{-5} \; \Omega\text{-cm}$$

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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.

$$\sigma = q\mu n = q(\mu_{e^-}+\mu_h)n_i = \sigma_0 \exp\left(-\frac{E_G}{2kT}\right)$$

$$\rho = \frac{1}{\sigma} = \rho_0 \exp\left(E_G/2kT\right)$$

at T=300K, $\rho = 50\ \Omega$-cm

$$\therefore \rho_0 = 50\exp\left(-\frac{0.66}{2\times8.62\times10^{-5}\times300}\right) = 1.54\times10^{-4}\ \Omega\text{-cm}$$

$\therefore$ at 1000K

$$\rho = 1.54\times10^{-4}\exp\left(\frac{0.66}{2\times1000\times8.62\times10^{-5}}\right) = 7.1\times10^{-3}\ \Omega\text{-cm}$$

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.

When $E_F = E_D$, $n = \frac{N_D}{2}$ [probability of finding an electron at the level $E_D$ (ie. that the level is occupied) is $\frac{1}{2}$]

$$\therefore \frac{N_D}{2} = N_D\exp\left(\frac{-0.007}{8.62\times10^{-5}\times T}\right)$$

So, $\ln\left(\frac{1}{2}\right) = -\frac{0.007}{8.62\times10^{-5}\times T} \Rightarrow T = 117\text{K}$